Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Easy access to new anthracenyl π-conjugates:Generation of distinct AIE-active materials

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Experimental Section

General Consideration: Reagents

All experiments were carried out in hot air oven–dried glasswares under nitrogen and argon atmosphere. 9-Arylanthracenylphosphonate was prepared in our lab using the recently published procedure [ref 8 in the manuscript].All aldehydes were purchased from Aldrich and Alfa-aesar. Bases KO^tBu and K_2CO_3 were purchased from Aldrich and used as received. THF was redistilled from sodium metal and benzophenone mixture. All other reagents were purchased from common suppliers and used without further purification. Column and flash chromatography were performed by using Silica gel 100-200 mesh and 230–400 mesh respectively. Reactions were monitored by thin–layer chromatography on pre-coated with silica gel 60 F_{254} plates (Merck & co.) and were visualized by UV- light (~365 nm).

Analytical Methods:

^1H, ^{13}C, ^{31}P-NMR spectra were recorded in $CDCl_3$ solution using Bruker Avance DRX (400 and 500 MHz). The signals were referenced to TMS and solvent used is deuterated chloroform (7.26 ppm in ^1H, 77.16 ppm ^{13}C). Chemical shifts are reported in ppm, multiplicities are indicated by s (singlet), d (doublet), t (triplet), dd (doublet of a doublet). Elemental analyses were carried out on a CHN analyser. The fluorescence spectra were recorded on a spectrofluorimeter. The electronic absorption spectra were recorded with JASCO-650V UV-Vis-NIR Scanning spectrophotometer. ESI-LCMS was recorded in Shimadzu LCMS-2020. The X-ray quality crystals of the compounds were grown by slow diffusion of n-hexane over CH_2Cl_2 solution. Single-crystal X-ray data were collected on an Enraf-Nonius MACH3 or on a Bruker AXS-SMART diffractometer using Mo Kα (λ= 0.71073 Å) radiation. The structures were solved by direct methods and refined by full-matrix least-squares method using standard procedures.[(a) Sheldrick, G. M. SADABS, Siemens Area Detector Absorption Correction; University of Go¨ttingen, Germany, 1996. (b) Sheldrick, G. M.SHELXTL NT, Crystal Structure Analysis Package, version 5.10; Bruker AXS, Analytical X-ray System: Madison, WI, 1999.]. Absorption corrections were done using SADABS program, where applicable. In general, all non-hydrogen atoms were refined anisotropically; hydrogen atoms were fixed by geometry or located by a difference Fourier map and refined isotropically. All bond angles, bond or other distances and dihedral angles are determined using mercury 3.3 software. DLS analyses were carried out with a Zetasizer Nano S from Malvern Instruments at 25°C. Time-resolved measurements were performed by using Time-correlated single-photon counting (TCSPC) spectrometer (Edinburgh, OB920)

with laser Diode source ($\lambda_{exc.}$ = 405 nm). A Dilute ludox solution in water was used to measure lamp profile. F900 decay analysis software was used to analysis the decay curves by using nonlinear least-squares iteration method. The quality of the fit was judged by the chi square (χ^2) values.Solid state quantum yields were calculated using SC-30 integrating sphere module on FS5 spectrofluorimeter (Edinburgh instruments). Fluorescence microscopic imaging studies were carried out under AxioImager M2 fluorescence microscope (Carl Zeiss, Germany). TGA was carried out on Shimadzu DTG-60 simultaneous DTA-TG Apparatus.

Absorption and emission spectra of compounds* 2a-e, 3a *in different solvents:

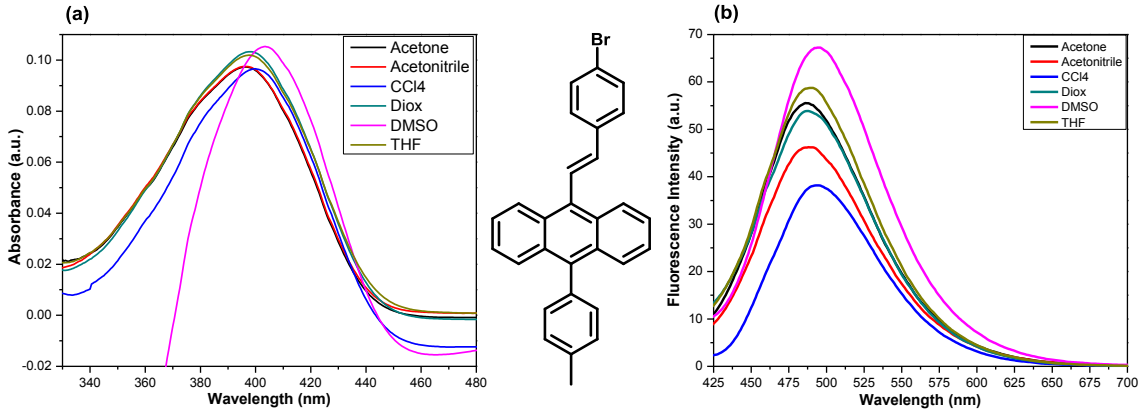

Fig S1 Compound **2a** (10^{-5}M) in various solvents (a) absorption spectra (b) emission spectra

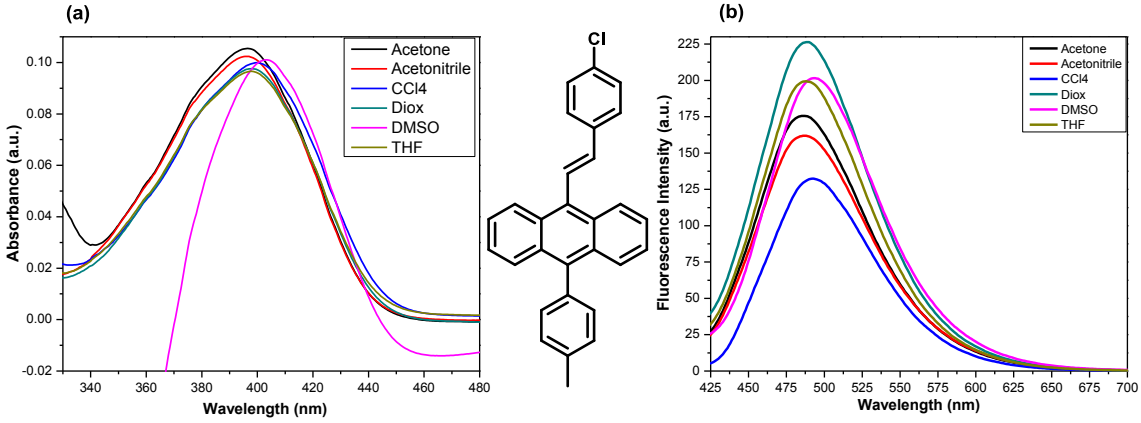

Fig S2 Compound **2b** (10^{-5}M) in various solvents (a) absorption spectra (b) emission spectra

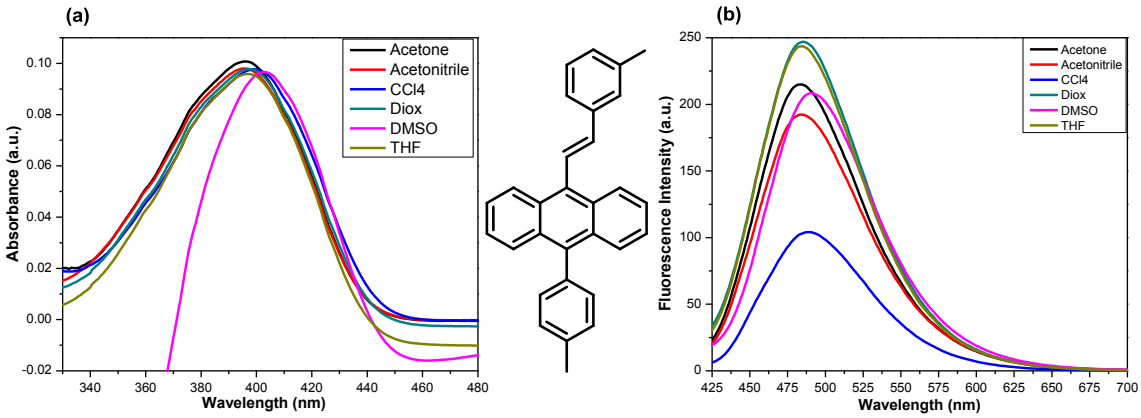

Fig S3 Compound **2c** (10^{-5}M) in various solvents (a) absorption spectra (b) emission spectra

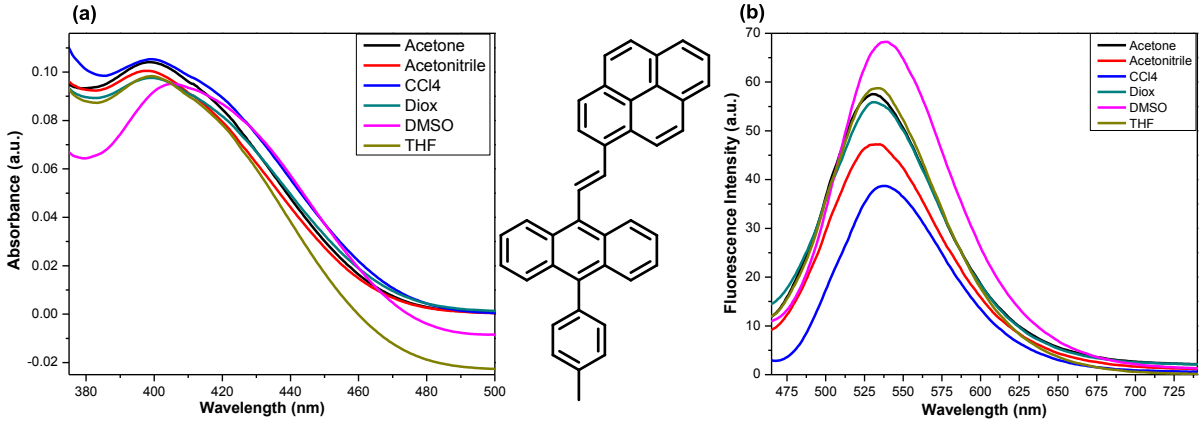

Fig S4 Compound **2d** (10^{-5}M) in various solvents (a) absorption spectra (b) emission spectra

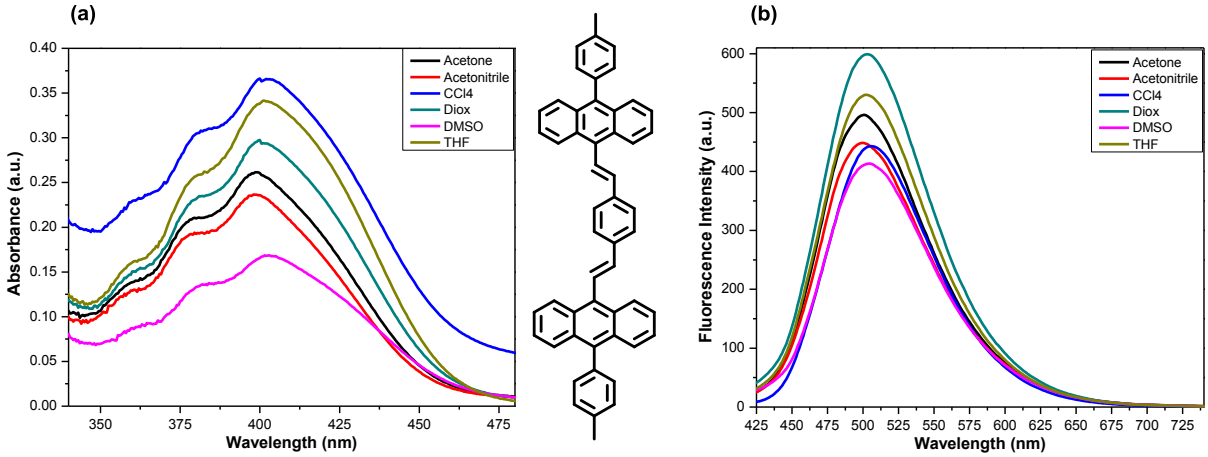

Fig S5 Compound **2e** (10^{-5}M) in various solvents (a) absorption spectra (b) emission spectra

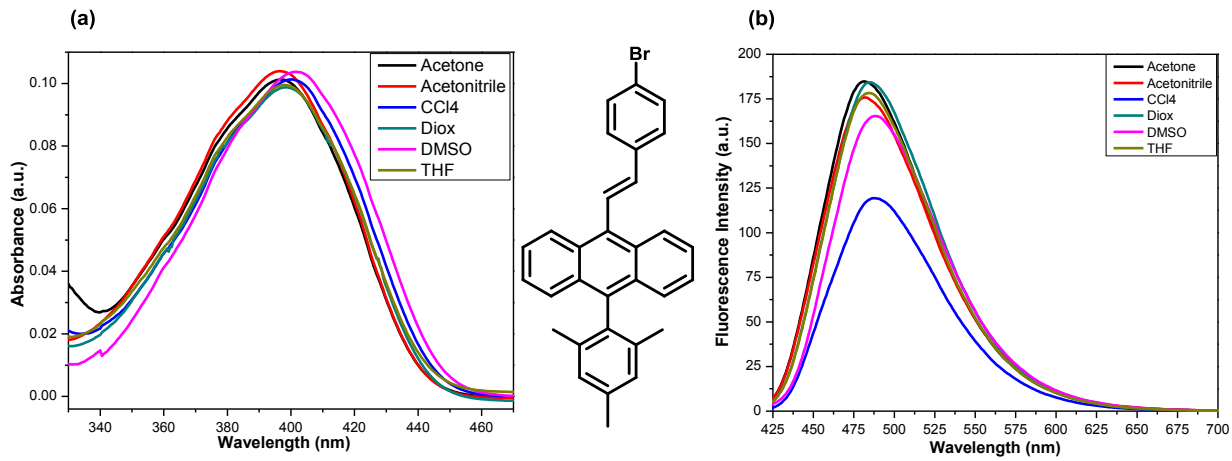

Fig S6 Compound **3a** (10^{-5}M) in various solvents (a) absorption spectra (b) emission spectra

Table S1: *Absorption wavelength maxima in different solvents*

Solvent	Abs λ_{max}2a	Abs λ_{max}2b	Abs λ_{max}2c	Abs λ_{max}2d	Abs λ_{max}2e	Abs λ_{max}3a
CCl_4	400	399.5	399	399	400	400
Diox	397.5	398	397.5	399	400	398.5
THF	398	398	397	399.5	401	398
Acetone	396.5	396.5	396	398.5	399	396.5
Acetonitrile	396	396	396	398	398	396.5
DMSO	403.5	403.5	403	405.5	401.5	401

Table S2: *Fluorescence emission maxima in different solvents*

Solvent	Emi λ_{max}2a	Emi λ_{max}2b	Emi λ_{max} 2c	Emi λ_{max}2d	Emiλ_{max}2e	Emi λ_{max}3a
CCl_4	495.5	494.5	489	540	506	488.5
Diox	494.5	493.5	489.5	545	503	490.5
THF	491.5	491.5	486	545.5	502	486.5
Acetone	491.5	491.5	489.5	542.5	501	485.5
Acetonitrile	494.5	490.5	487	542	499	487
DMSO	500.5	498	494.5	540.5	505	490.5

Table S3: *Quantum yields of compounds in different solvents with reference to quinine sulphate in 0.1M H_2SO_4 (error ± 10%)*

Solvent	Φ_{F2a}	Φ_{F2b}	Φ_{F2c}	Φ_{F2d}	Φ_{F2e}	Φ_{F3a}
CCl_4	0.2	0.26	0.22	0.07	0.25	0.2
Dioxane	0.22	0.36	0.43	0.07	0.38	0.22

DMSO	0.24	0.4	0.48	0.12	0.45	0.22
Acetone	0.19	0.28	0.34	0.05	0.33	0.23
Acetonitrile	0.2	0.3	0.39	0.07	0.39	0.21
THF	0.18	0.27	0.34	0.05	0.25	0.26
Solid state	0.02	0.02	0.03	0.01	0.01	0.03

Table S4: *DLS studies to obtain average particle size for the aggregates*

Compound	d.nm
2f	95.03
4a	161.0
4b	111.5
5	86.65

Absorption and emission spectra of compound* 2e *in molecular and aggregate forms showing aggregation caused quenching (ACQ)

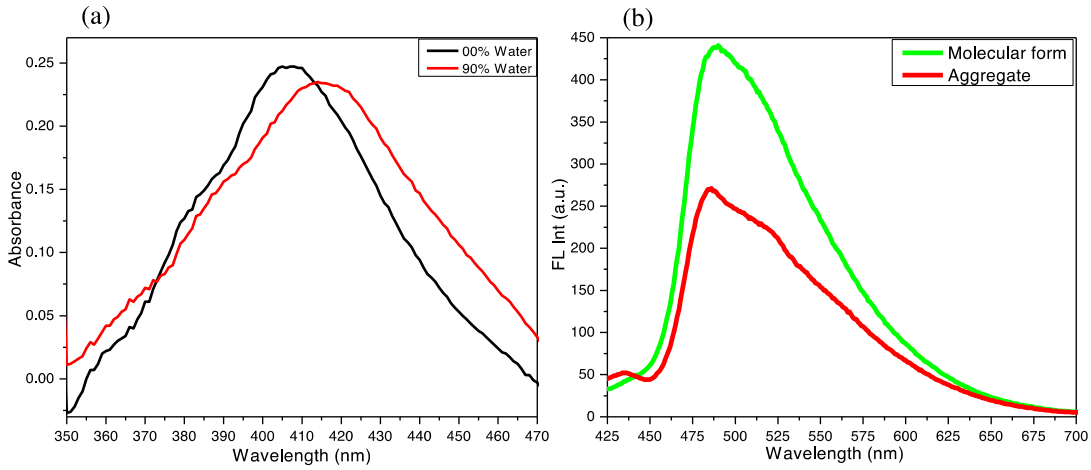

Fig S7 Compound **2e** (10^{-5}M) as molecular form (in MeCN) & aggregate form (in 90% Water in MeCN) (a) absorption spectra (b) emission spectra

Absorption spectra of compound* 4a *in molecular and aggregate forms

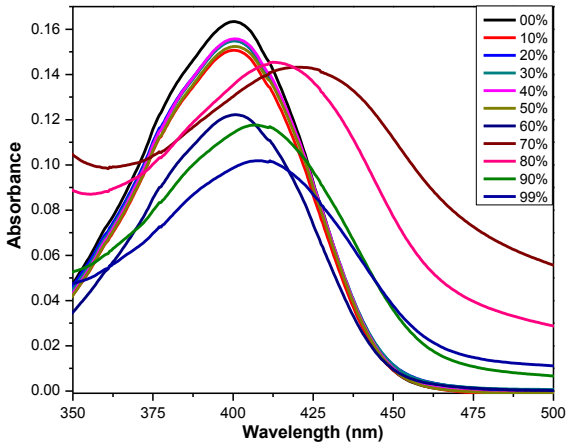

Fig S8 The absorption spectra of compound **4a** (10^{-5}M) in 1,4-dioxane with water fractions

AIE effect using MeOH in the place of water as a polar solvent: Polarity effect

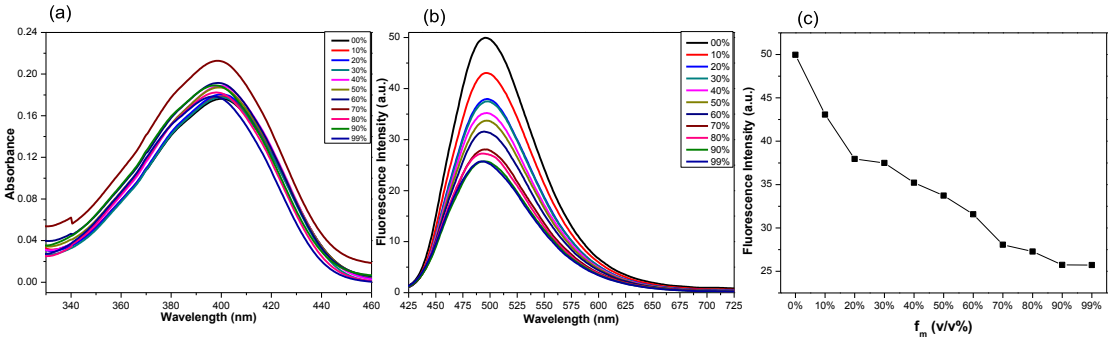

Fig S9 Compound **4a** (10^{-5}M) in 1,4-dioxane with MeOH fractions (a) absorption spectra (b) emission spectra (c) decrease of Fl. intensity with the increase of methanol fractions in 1,4-dioxane.

AIE effect studies using anthracene

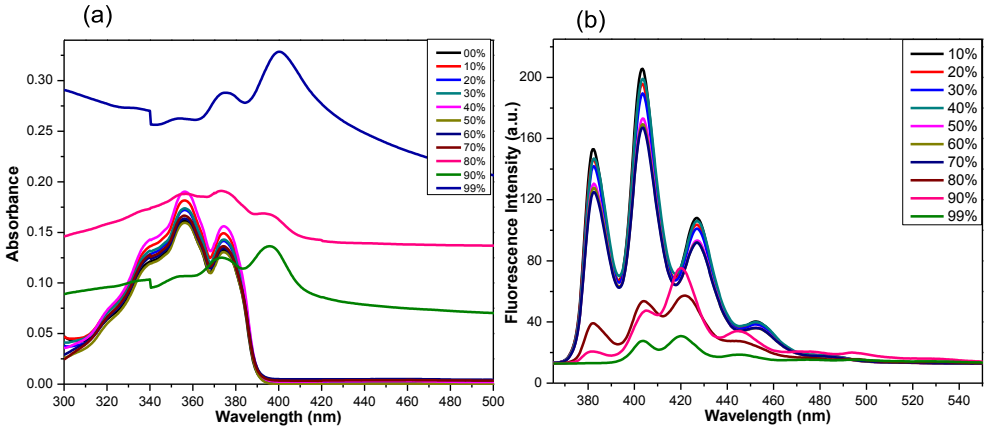

Fig S10 Anthracene(10^{-5}M) in Dioxane with water fractions (a) absorption spectra (b) emission spectra

***Time-resolved fluorescence studies (life time decay experiment) on compound* 4a**

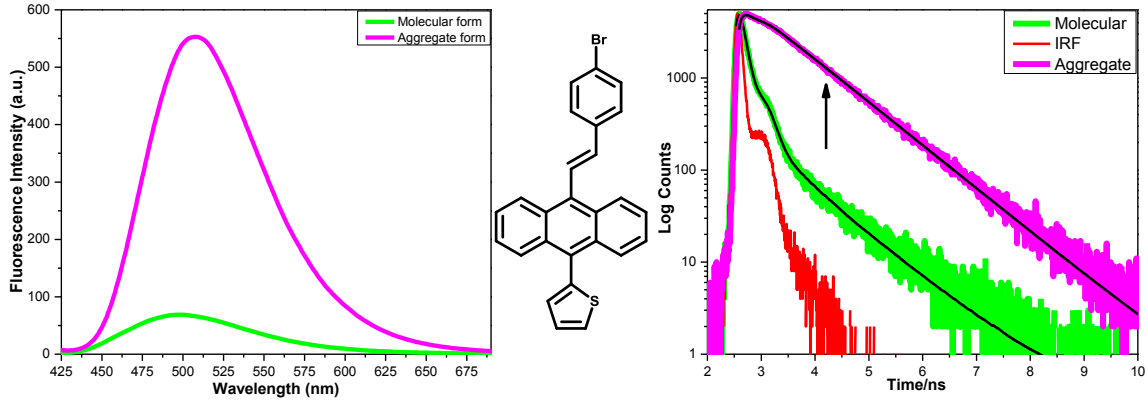

Fig S11 Compound **4a** (10^{-5}M) in 1,4-dioxane (a) emission spectra (b) lifetime decay plot of **4a** in molecular and aggregate forms. (λ_{ex} = 405 nm)

Viscochromism experiment:

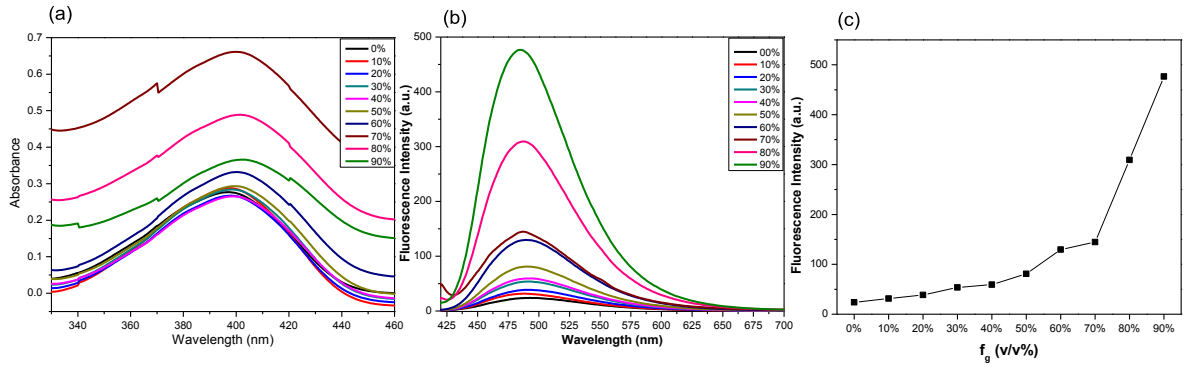

Fig S12 Compound **4a** (10^{-5} M) in MeOH with glycerol fractions showing viscochromism (a) absorption spectra (b) emission spectra (c) glycerol fractions in MeOH. (λ_{ex} = 405 nm)

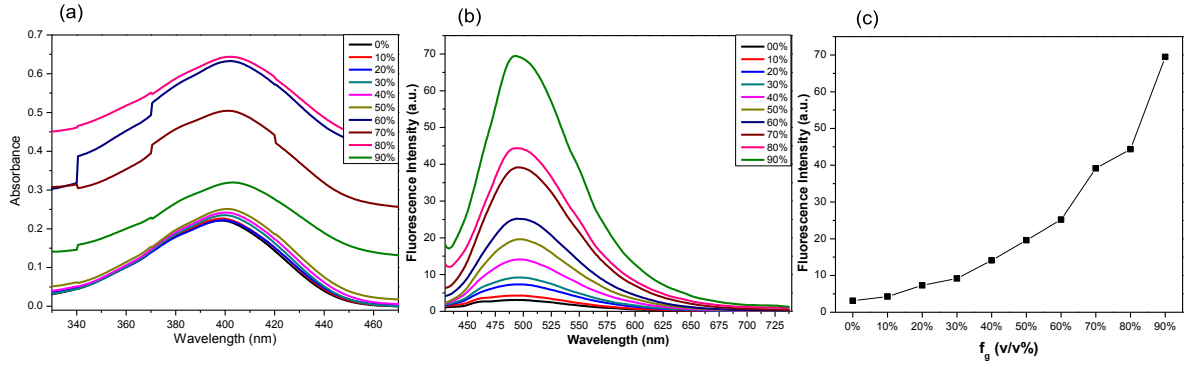

Fig S13 Compound **4c** (10^{-5} M) in MeOH with glycerol fractions showing viscochromism (a) absorption spectra (b) emission spectra (c) glycerol fractions in MeOH. (λ_{ex} = 405 nm)

***P-XRD patterns for compounds* 3a *and* 4b:**

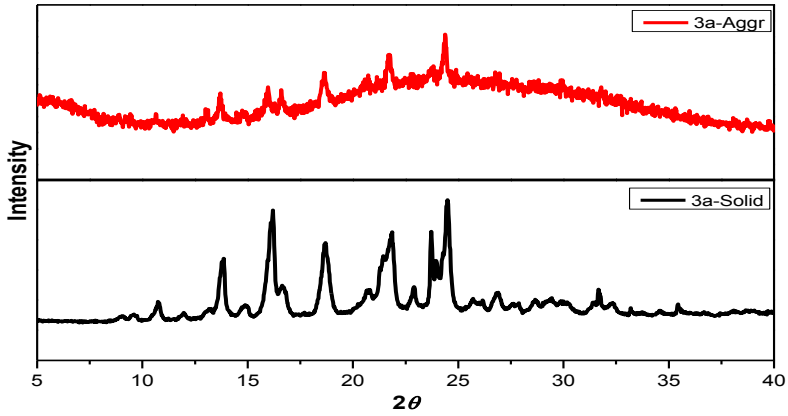

Fig S14 P-XRD patterns of as prepared (solid) and aggregates of compound **3a**.

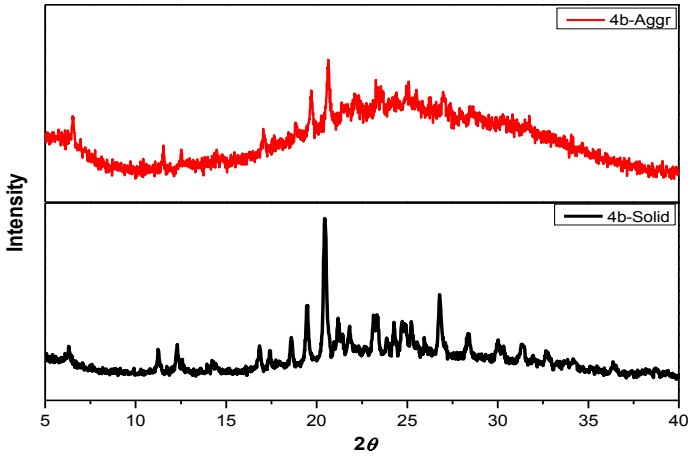

Fig S15 P-XRD patterns of as prepared (solid) and aggregates of compound **4b**.

***AIE studies on compounds* 4b-c**

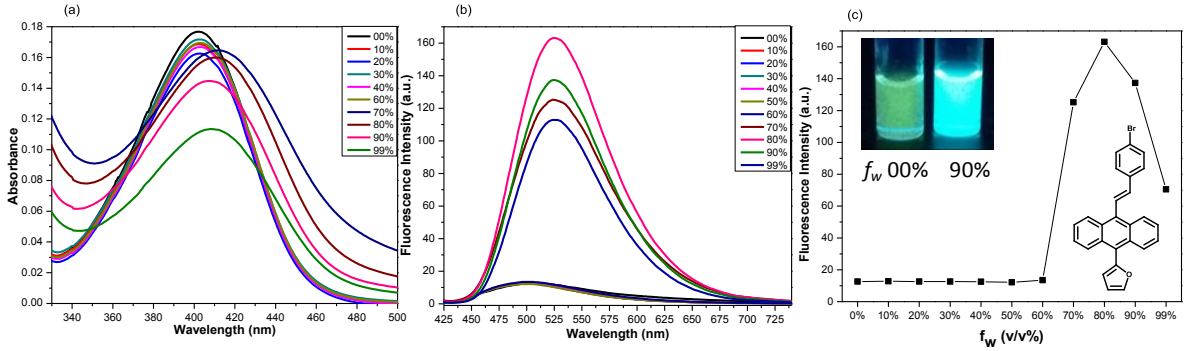

Fig S16 Compound **4b** (10^{-5}M) in acetonitrile (a) absorption spectra (b) emission spectra and (c) water fractions plot showing AIEE, inset images of **4b** molecular form (in acetonitrile) and aggregate form (in 90% water in acetonitrile). (λ_{ex} = 405 nm)

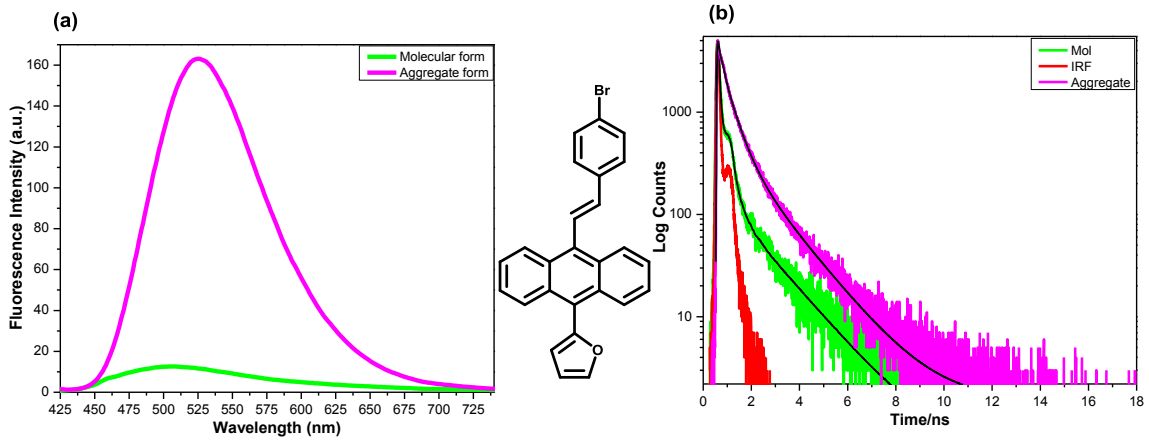

Fig S17 Compound **4b** (10^{-5}M) in acetonitrile (a) emission spectra (b) lifetime decay plot of **4b** in molecular and aggregate forms. (λ_{ex} = 405 nm)

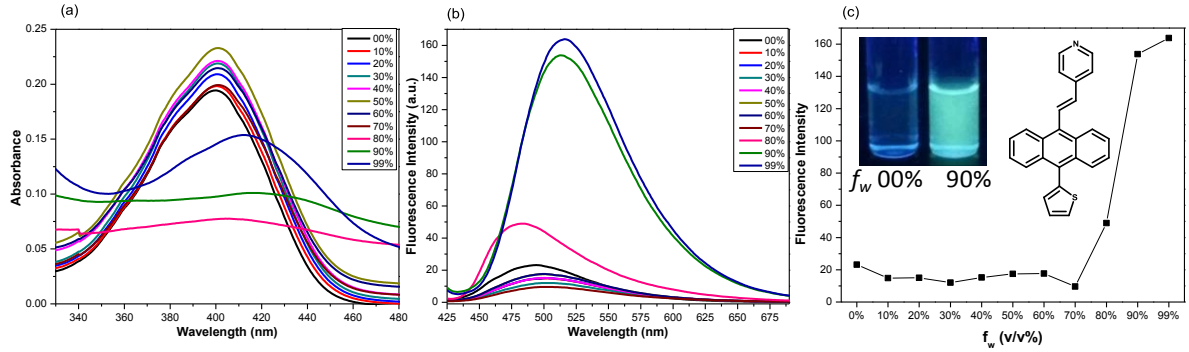

Fig S18 Compound **4c** (10^{-5}M) in 1,4-dioxane (a) absorption spectra (b) emission spectra and (c) water fractions plot showing AIEE, inset images of **4c** molecular form (in 1,4-dioxane) and aggregate form (in 90% water in 1,4-dioxane). (λ_{ex} = 405 nm)

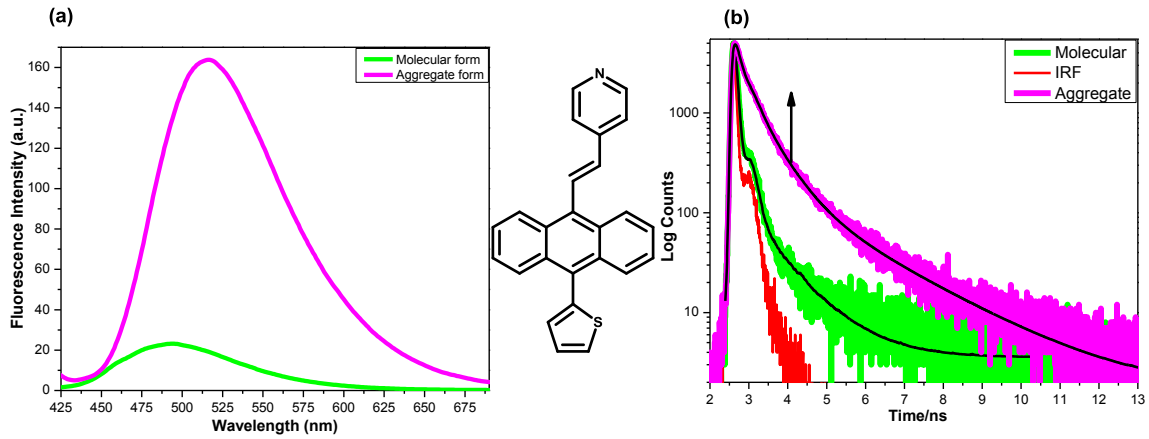

Fig S19 Compound **4c** (10^{-5}M) in 1,4-dioxane (a) emission spectra (b) lifetime decay plot of **4c** in molecular and aggregate forms. (λ_{ex} = 405 nm)

AIE studies on compound **2f** *and* **2g**

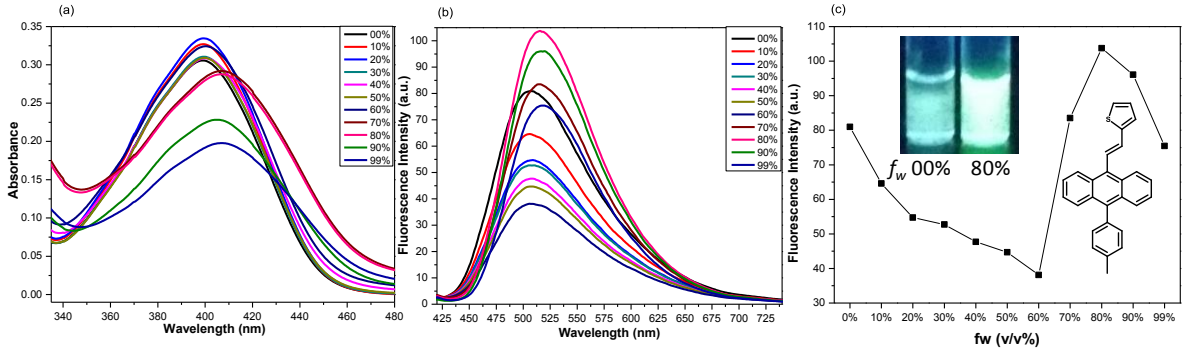

Fig S20 Compound **2f** (10^{-5}M) in acetonitrile (a) absorption spectra (b) emission spectra and (c) water fractions plot showing AIEE, inset images of **2f** molecular form (in acetonitrile) and aggregate form (80% water in acetonitrile). (λ_{ex} = 405 nm)

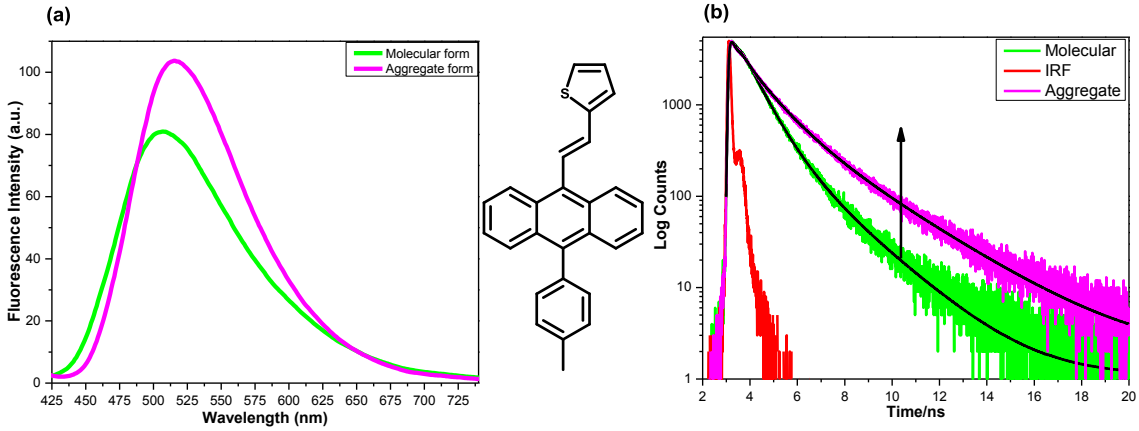

Fig S21 Compound **2f** (10^{-5}M) in acetonitrile (a) emission spectra (b) lifetime decay plot of **2f** in molecular and aggregate forms. (λ_{ex} = 405 nm)

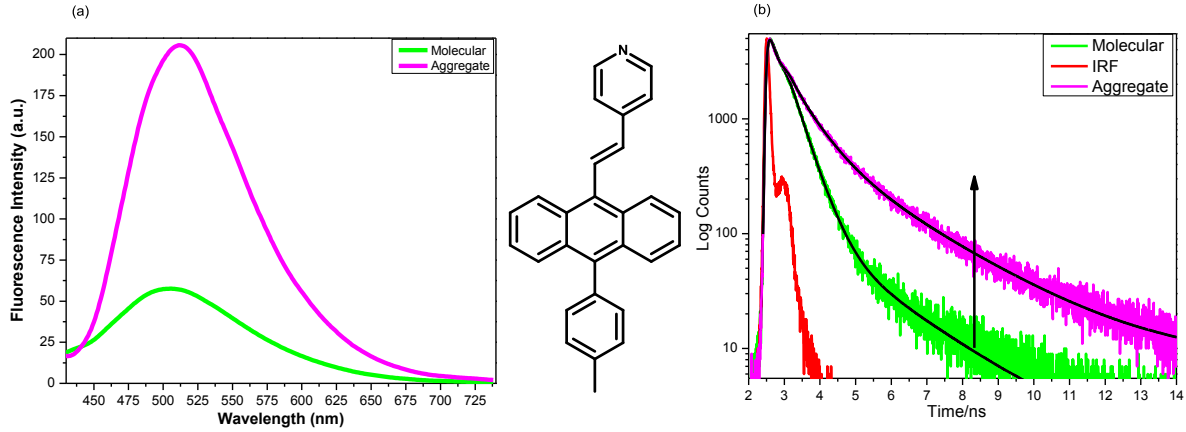

Fig S22 Compound **2g** (10^{-5}M) in acetonitrile (a) emission spectra (b) lifetime decay plot of **2g** in molecular and aggregate forms. (λ_{ex} = 405 nm)

***P-XRD pattern for compound* 2f:**

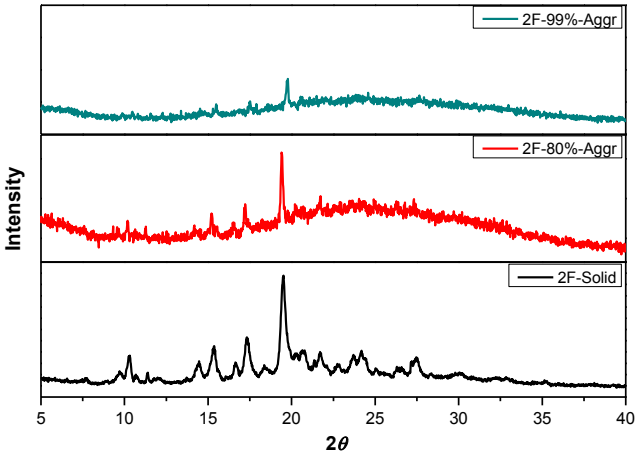

Fig S23 P-XRD patterns of as prepared (solid) and aggregates of compound **2f**.

Thermal stability: Thermogravimetric analysis data for few compounds:

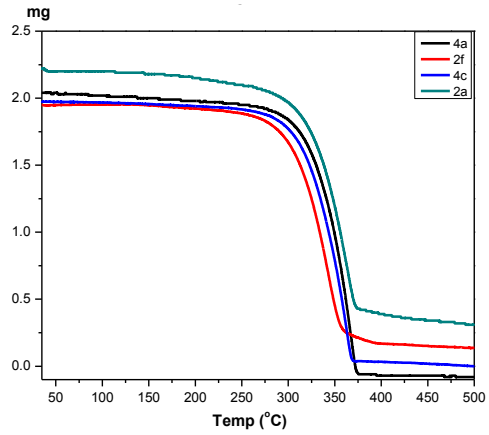

Fig S24 Thermogravimetric analysis of compounds **4a**, **2f**, **4c**, **2a**

AIE studies on compound 5:

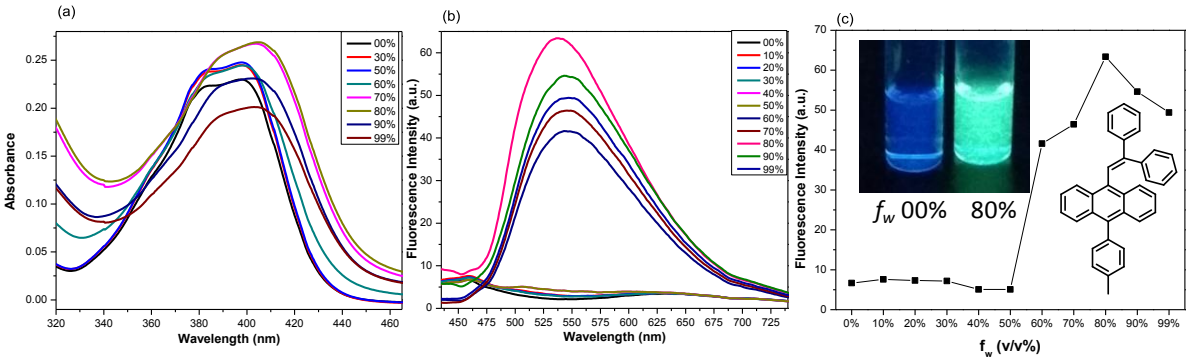

Fig S25 Compound **5** (10^{-5}M) in acetonitrile (a) Absorption spectra (b) Emission spectra and (c) water fractions plot showing AIEE, inset images of **5** molecular form (in acetonitrile) and aggregate form (in 80% water in acetonitrile). (λ_{ex} = 405 nm)

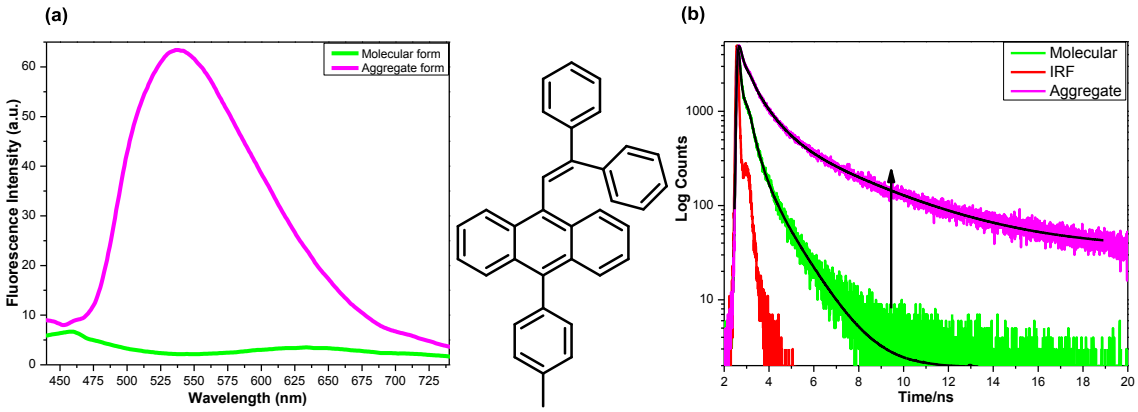

Fig S26 Compound **5** (10^{-5} M) in acetonitrile (a) Emission spectra (b) Lifetime decay plot of **5** in molecular and aggregate forms. (λ_{ex} = 405 nm)

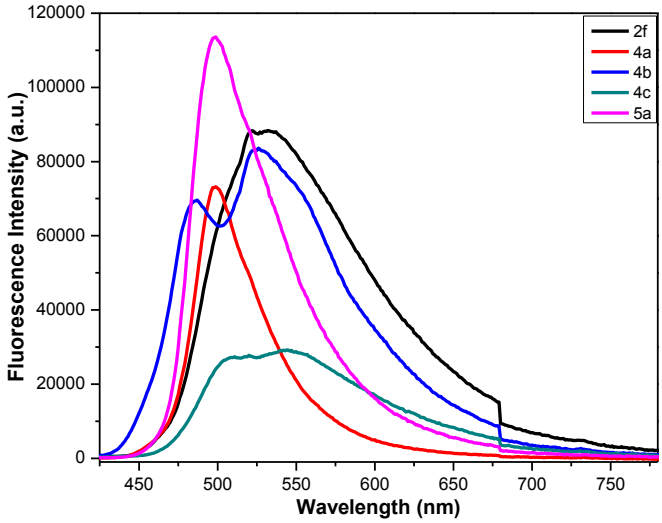

Fig S27 Solid state fluorescence of AIEE active compounds

Molecular structures for compounds 3a and 4b

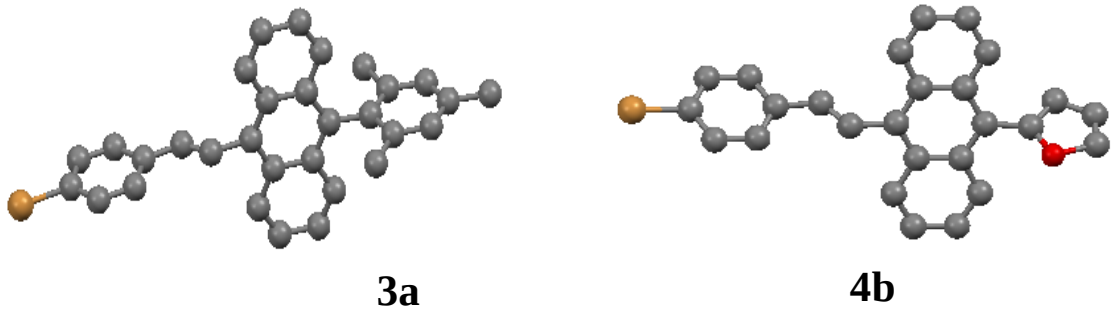

Fig S28 Molecular structures for compounds **3a** and **4b**

Table S5: Lifetime decay profile with individual exponentials and quantum yields

Compound	Form	B_1'	B_2'	B_3'	τ_1(ns)	τ_2(ns)	τ_3(ns)	<τ>(ns)	χ^2	Φ_F (%) [a]
2f	Molecular	0.9	0.1	--	0.74	1.92	--	0.86	1.08	4.63
	Aggregate	0.39	0.46	0.15	0.28	1.08	2.67	1.00	1.07	9.50
	Solid state	0.4	0.32	0.28	0.1	0.79	1.96	0.84	1.14	2.98
2g	Molecular	0.98	0.02	--	0.39	2.01	--	0.42	1.15	3.19
	Aggregate	0.52	0.39	0.09	0.17	0.66	2.24	0.55	1.07	8.01
	Solid state	0.75	0.25	--	0.75	2.59	--	1.21	1.14	4.53
4a	Molecular	0.98	0.02	--	0.09	0.93	--	0.11	1.03	0.81
	Aggregate	1.00	--	--	0.92	--	--	0.93	1.14	13.70
	Solid state	0.5	0.5	--	0.69	1.37	--	1.03	1.04	3.96
4b	Molecular	0.95	0.04	0.01	0.03	0.22	1.6	0.05	1.08	0.68
	Aggregate	0.56	0.37	0.07	0.23	1.11	3.7	0.80	1.19	5.52
	Solid state	0.32	0.64	0.04	0.13	0.5	1.7	0.43	1.04	3.52
4c	Molecular	0.989	0.01	0.001	0.04	0.35	2.7	0.04	1.17	0.75
	Aggregate	0.71	0.26	0.03	0.15	0.53	1.94	0.30	1.08	6.19
	Solid state	0.59	0.31	0.1	0.46	2.18	7.68	1.71	1.15	1.34
5	Molecular	0.87	0.11	0.02	0.04	0.3	1.1	0.09	1.16	0.05
	Aggregate	0.76	0.21	0.03	0.03	1.5	7.70	0.57	1.13	35.13
	Solid state	0.55	0.45	--	0.49	2.2	--	1.26	1.18	6.62

[a]error: ± 10%

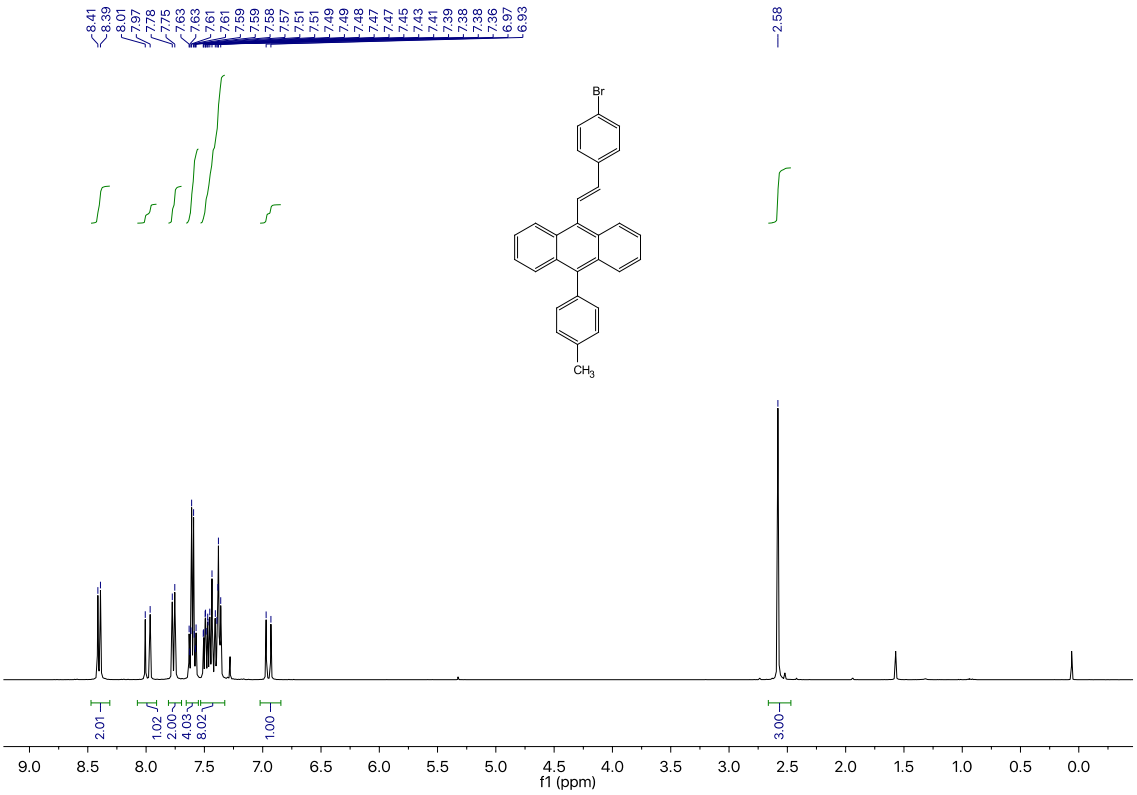

Fig S29 ^{1}H-NMR of compound **2a**

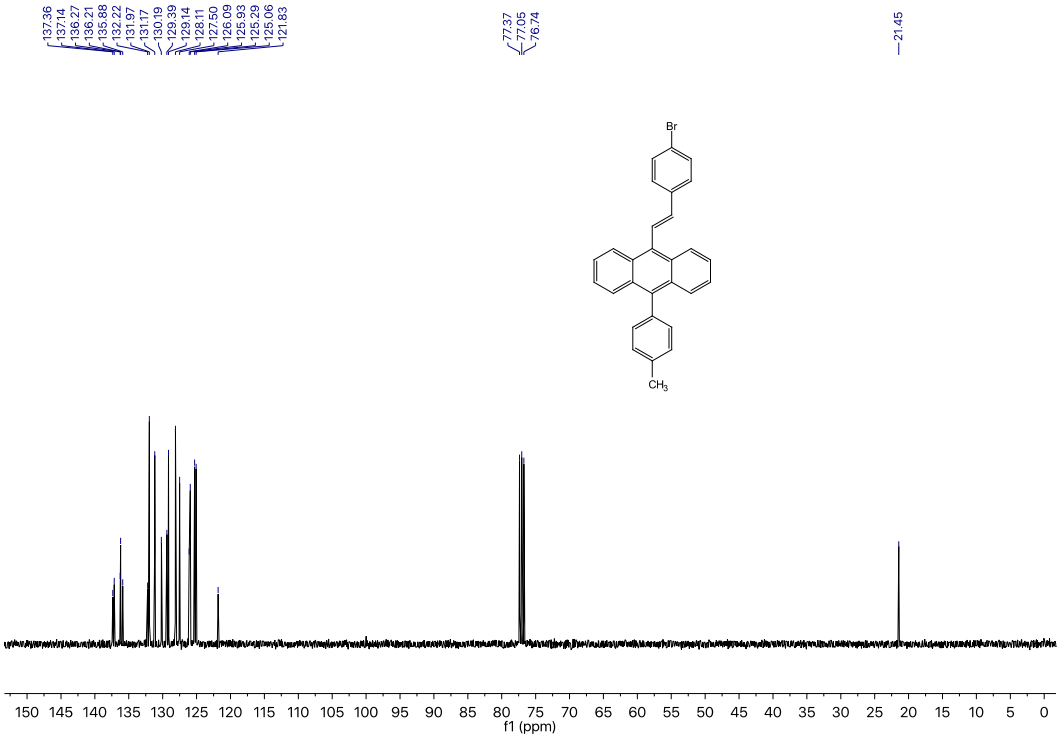

Fig S30 ^{13}C-NMR of compound **2a**

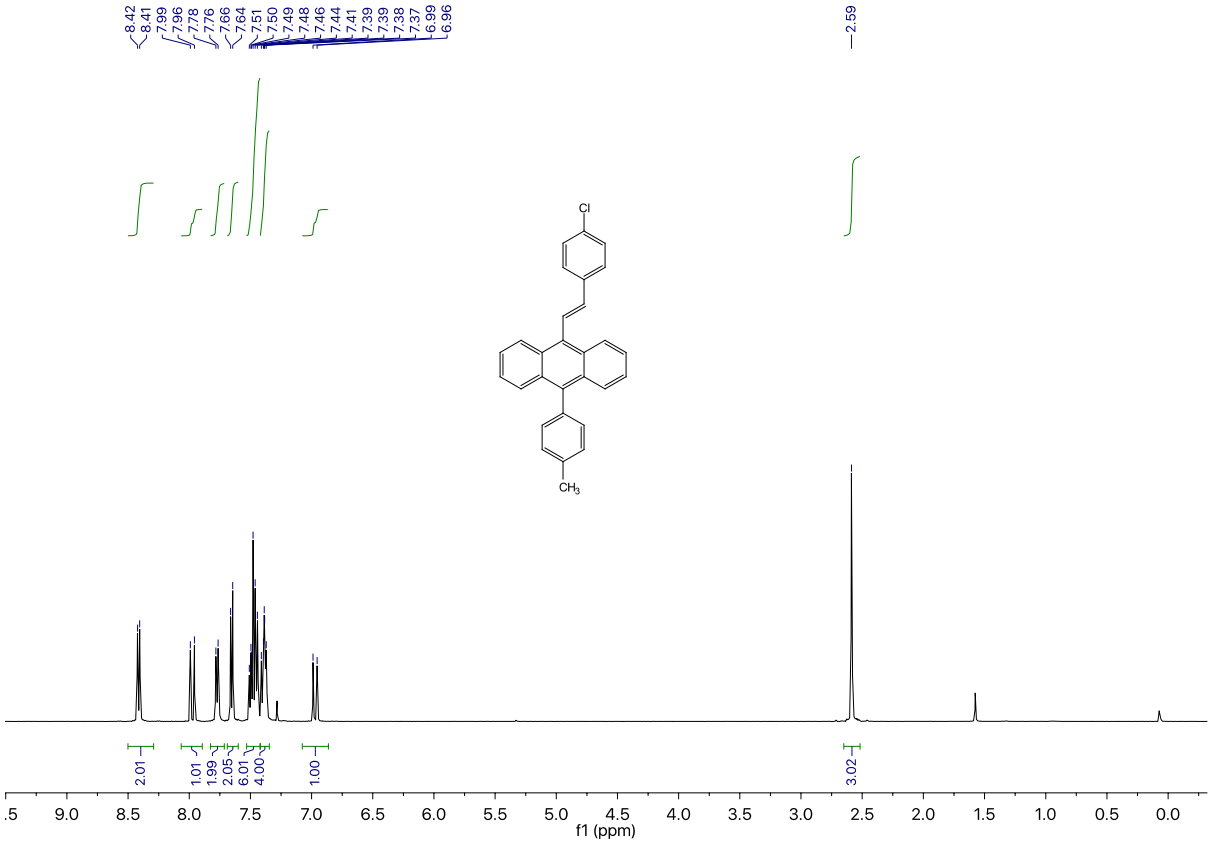

Fig S31 ^{1}H-NMR of compound **2b**

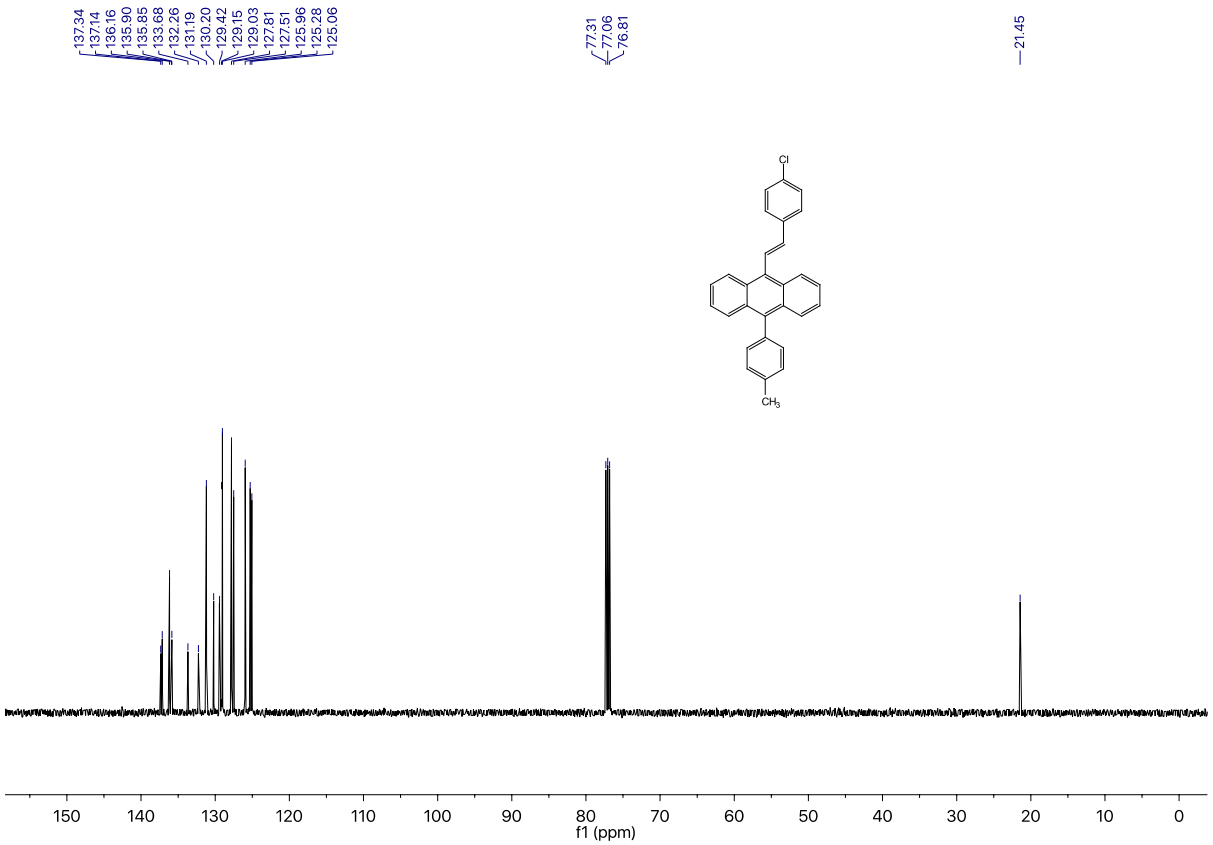

Fig S32 ^{13}C-NMR of compound **2b**

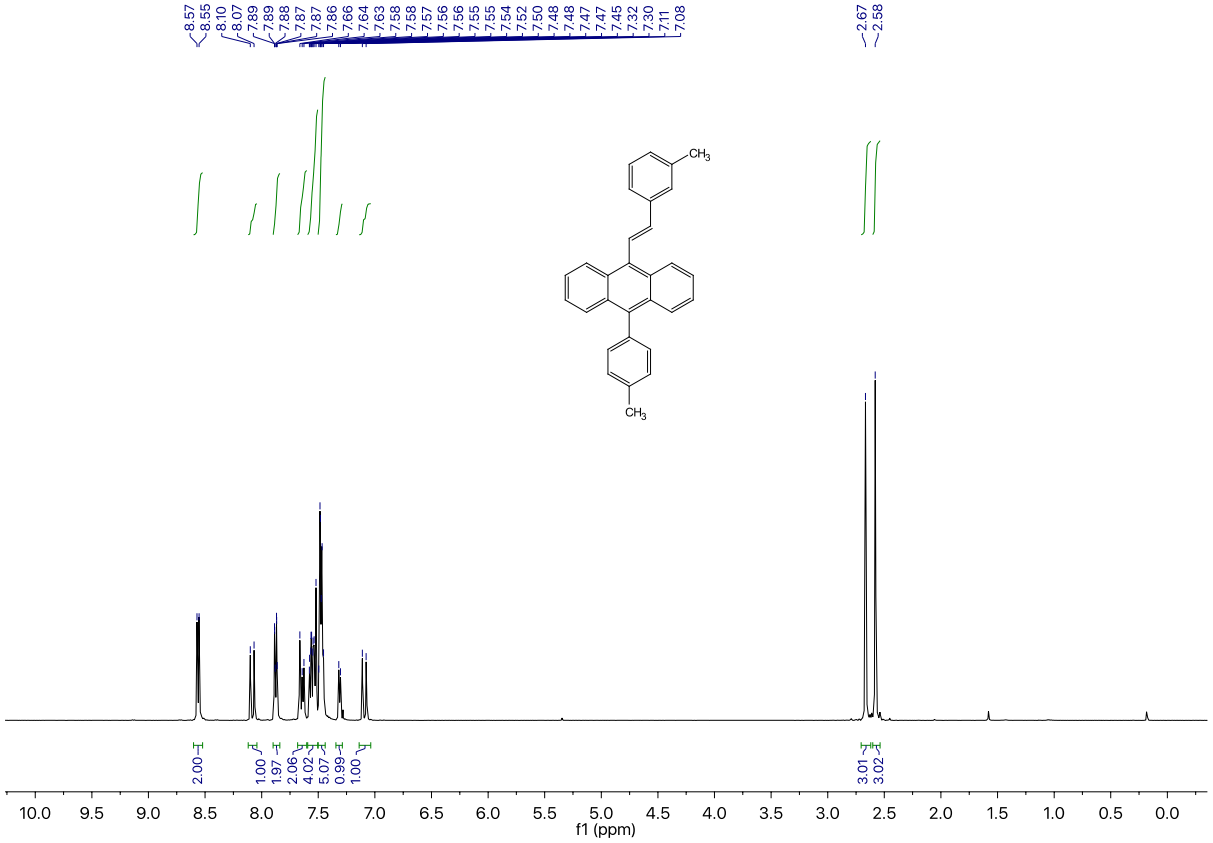

Fig S33 ^{1}H-NMR of compound **2c**

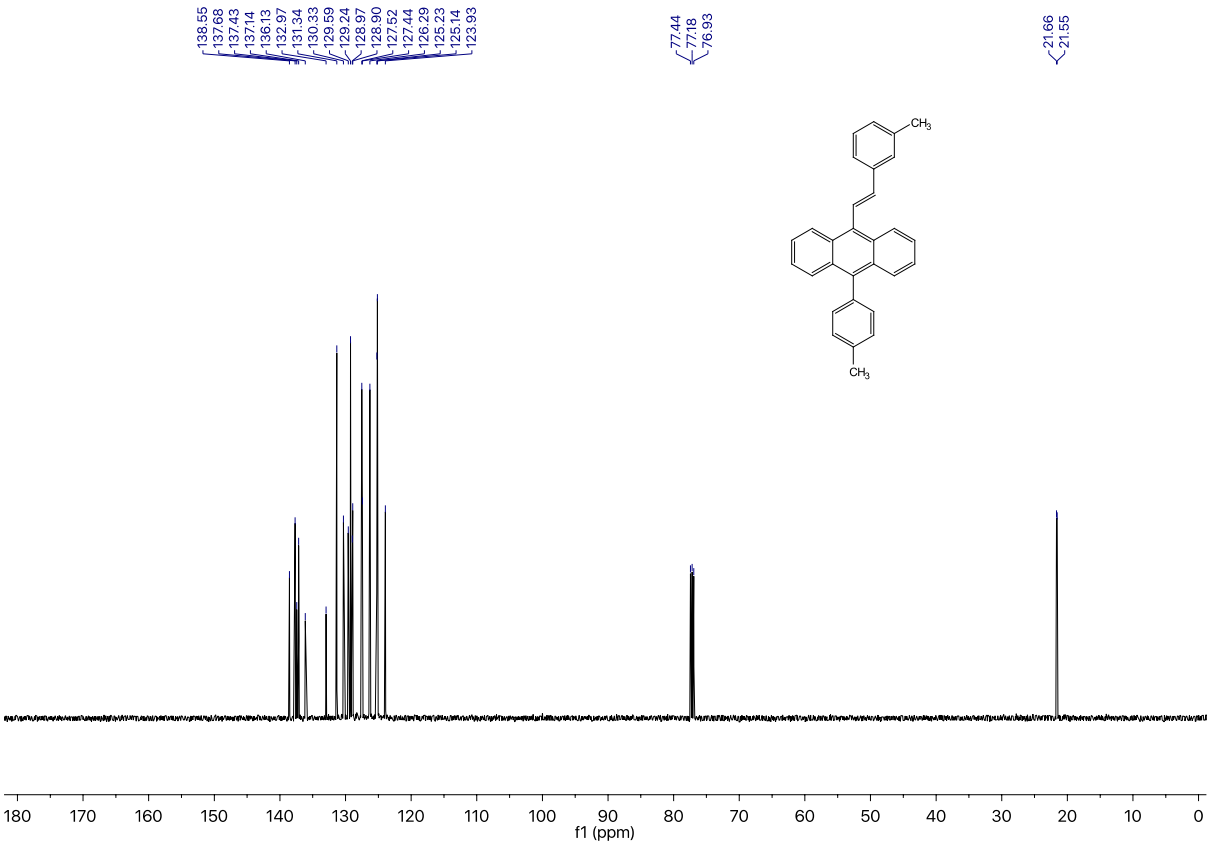

Fig S34 ^{13}C-NMR of compound **2c**

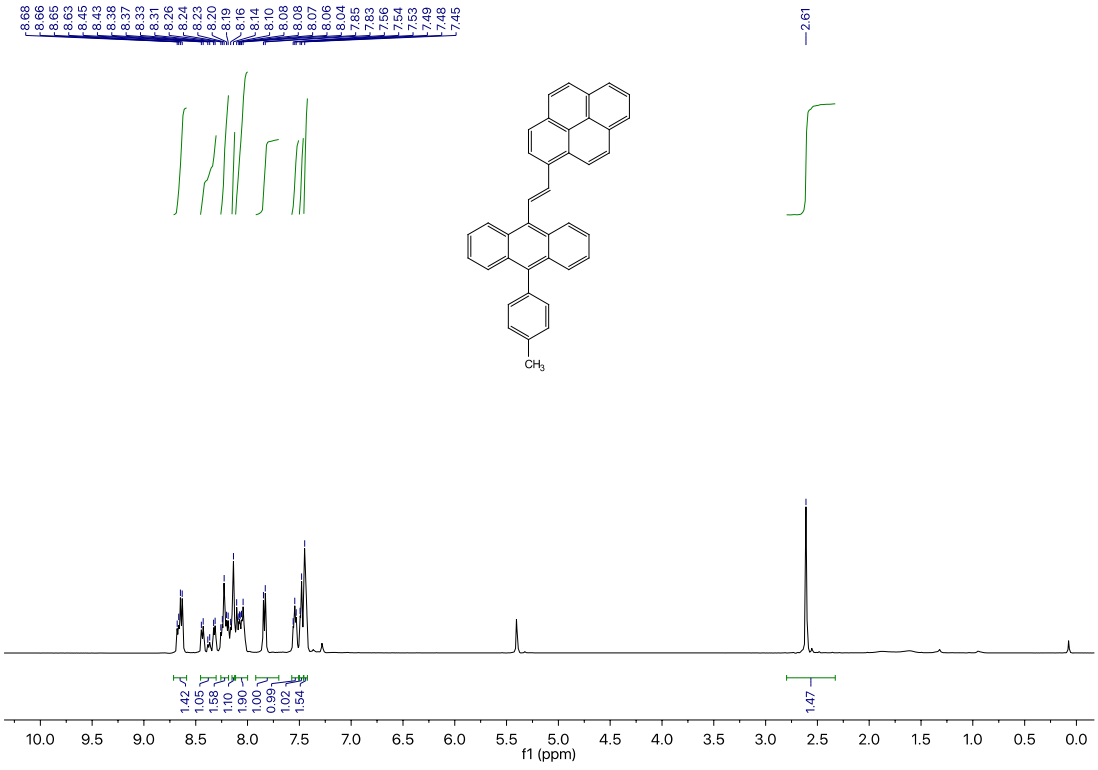

Fig S35 ^{1}H-NMR of compound **2d**

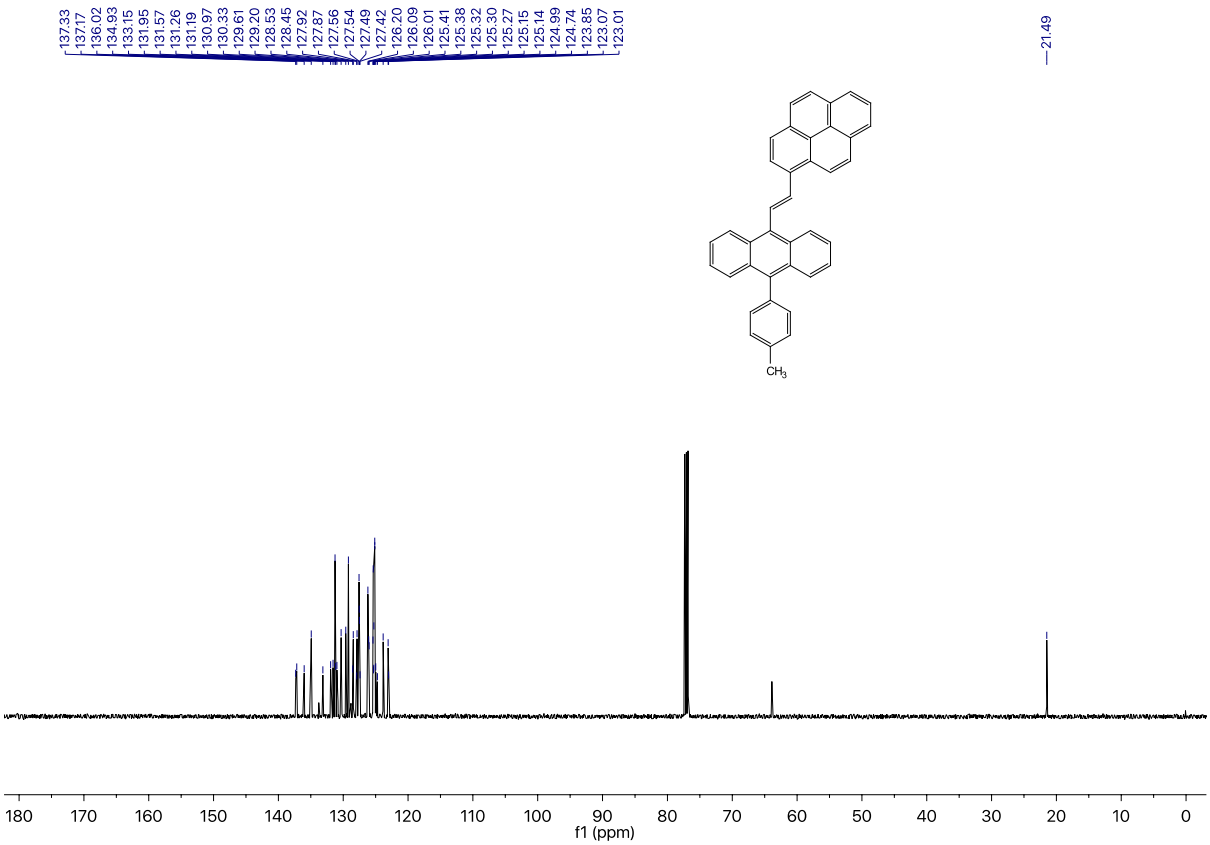

Fig S36 ^{13}C-NMR of compound **2d**

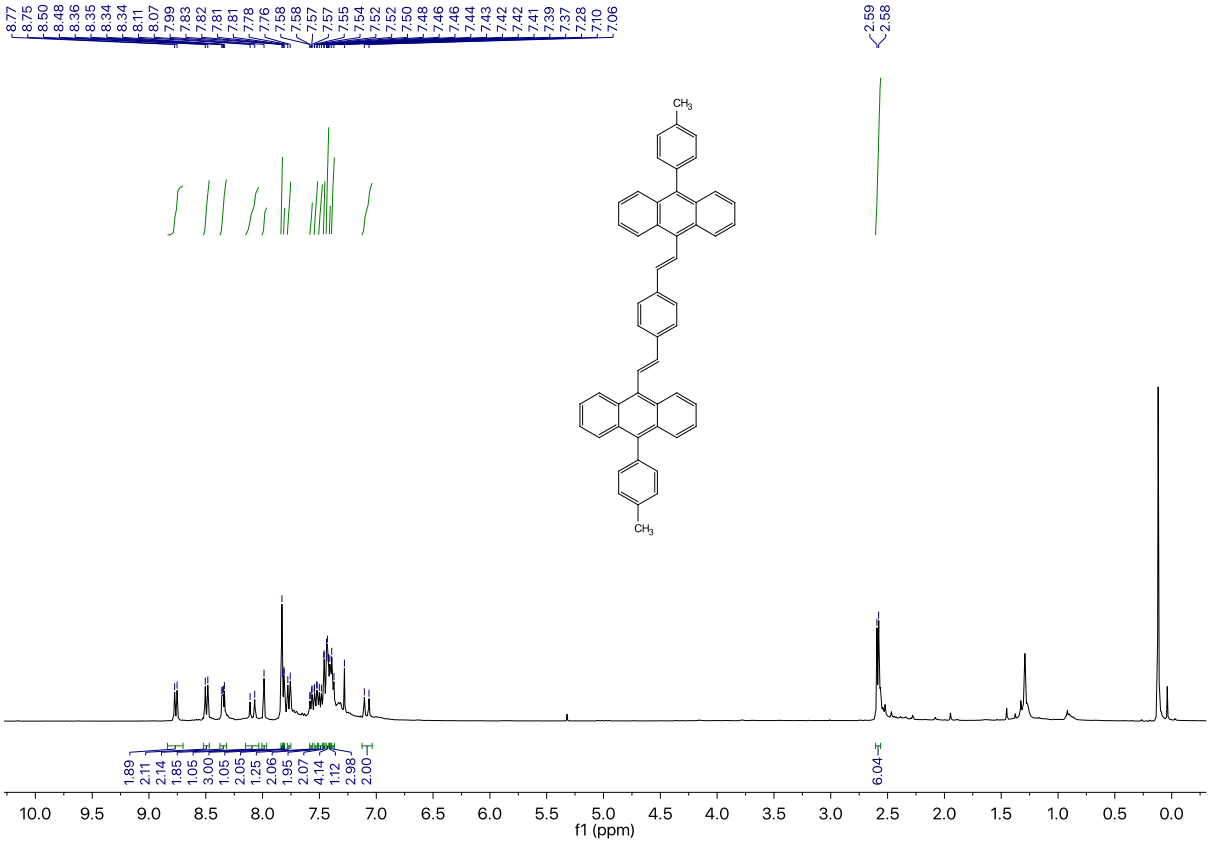

Fig S37 ^{1}H-NMR of compound **2e**

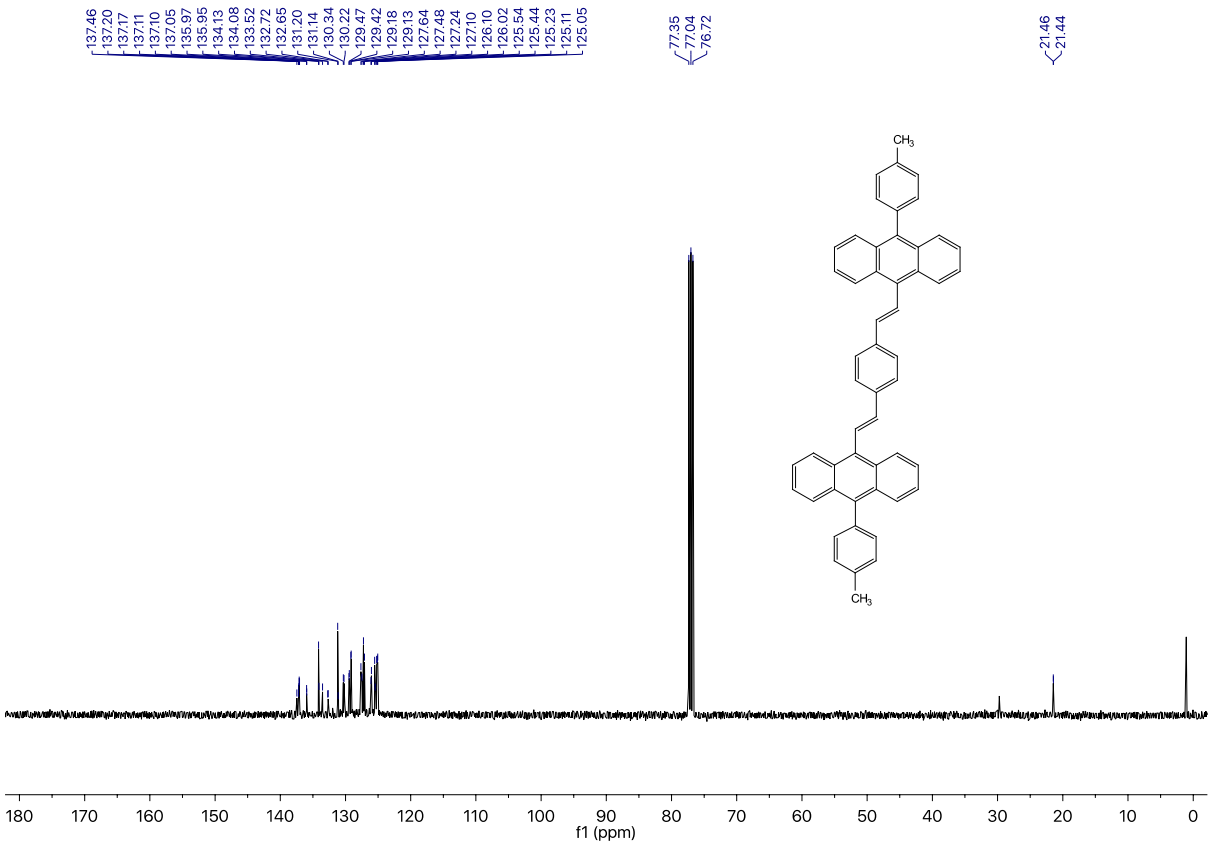

Fig S38 ^{13}C-NMR of compound **2e**

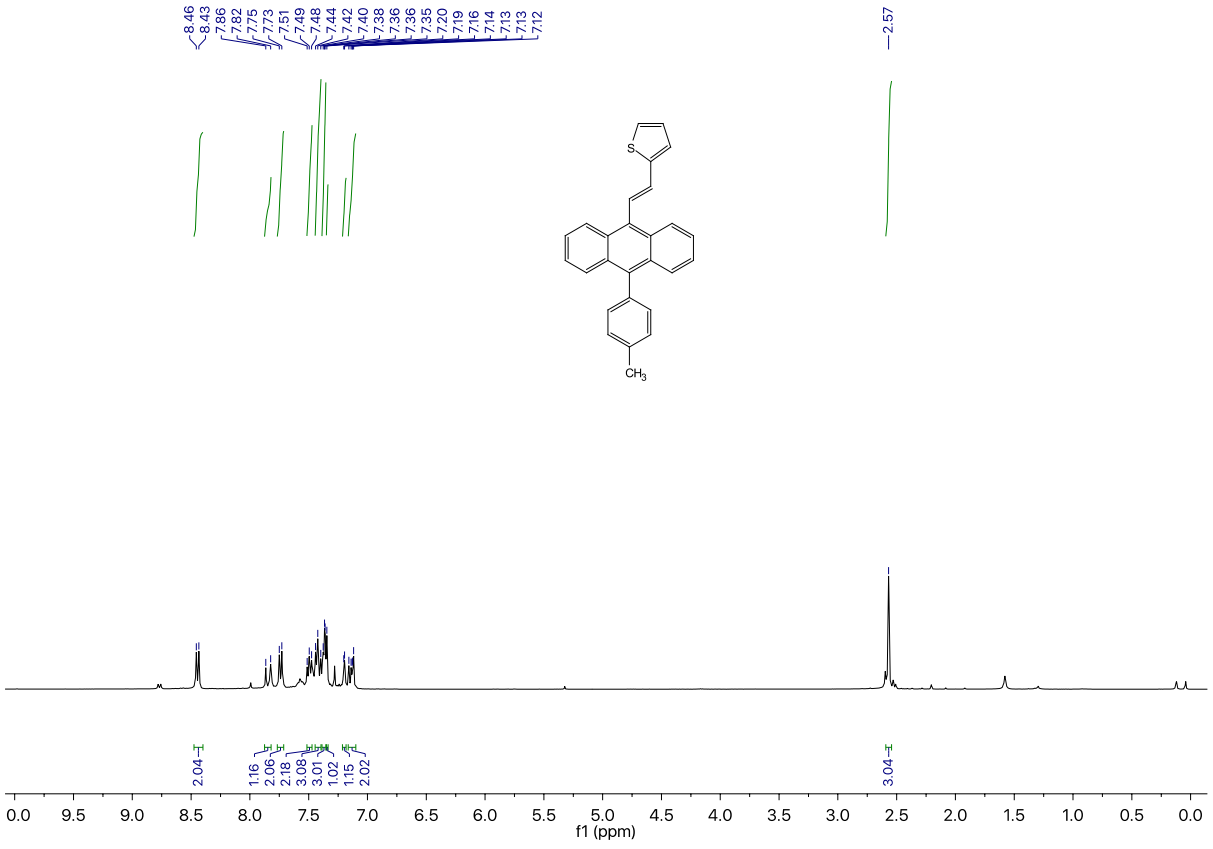

Fig S39 ^{1}H-NMR of compound **2f**

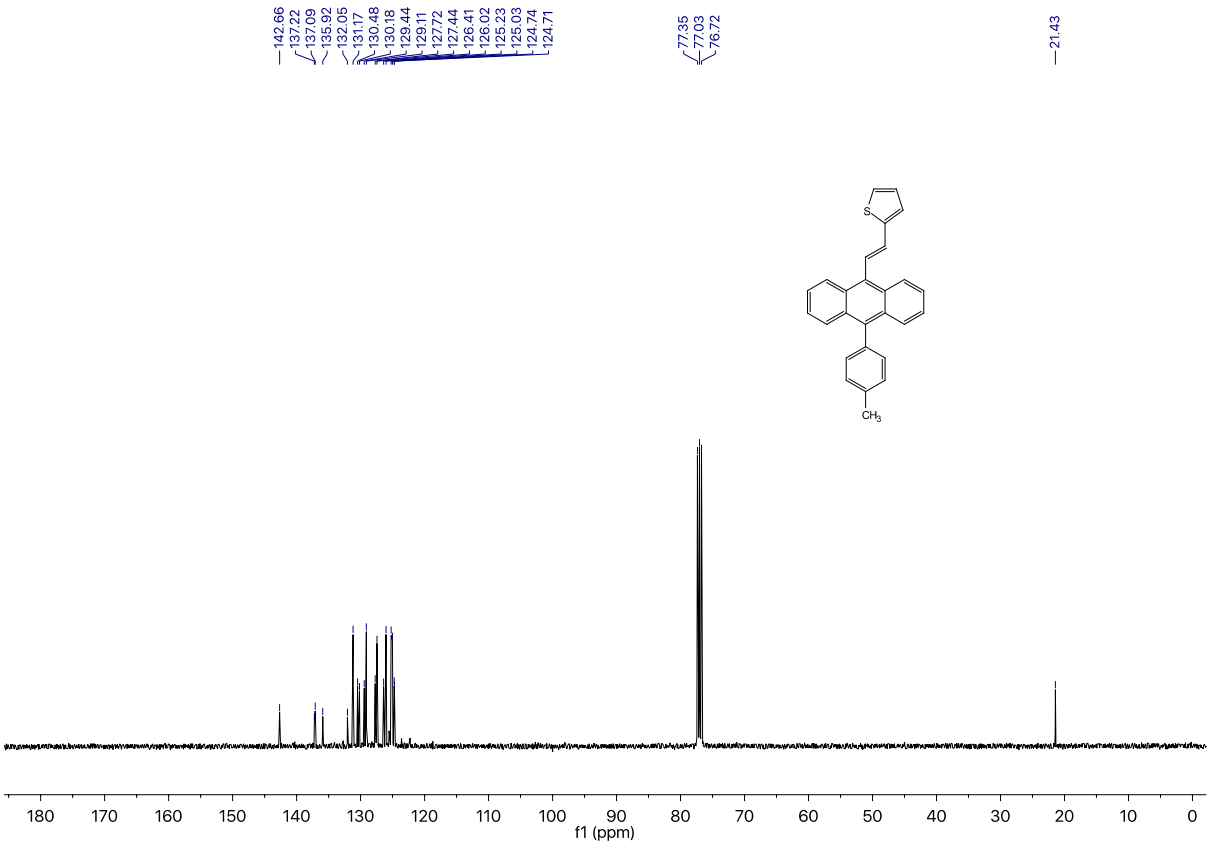

Fig S40 ^{13}C-NMR of compound **2f**

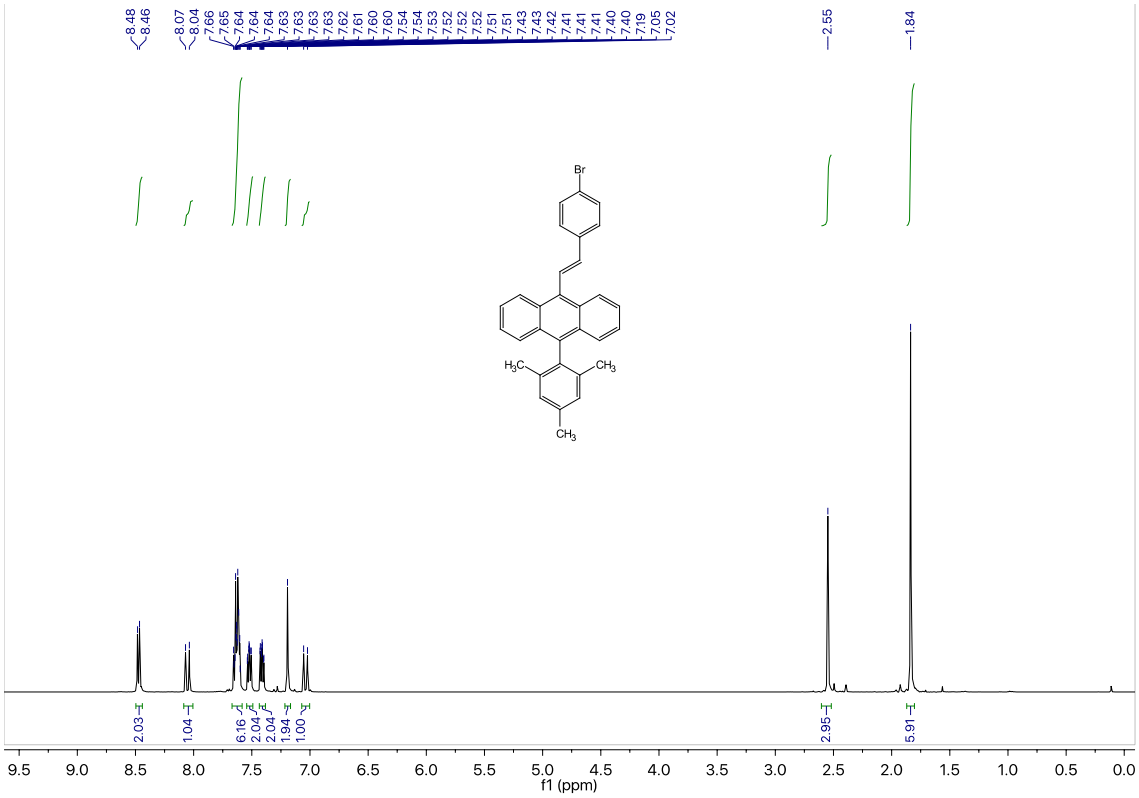

Fig S41^{1}H-NMR of compound **3a**

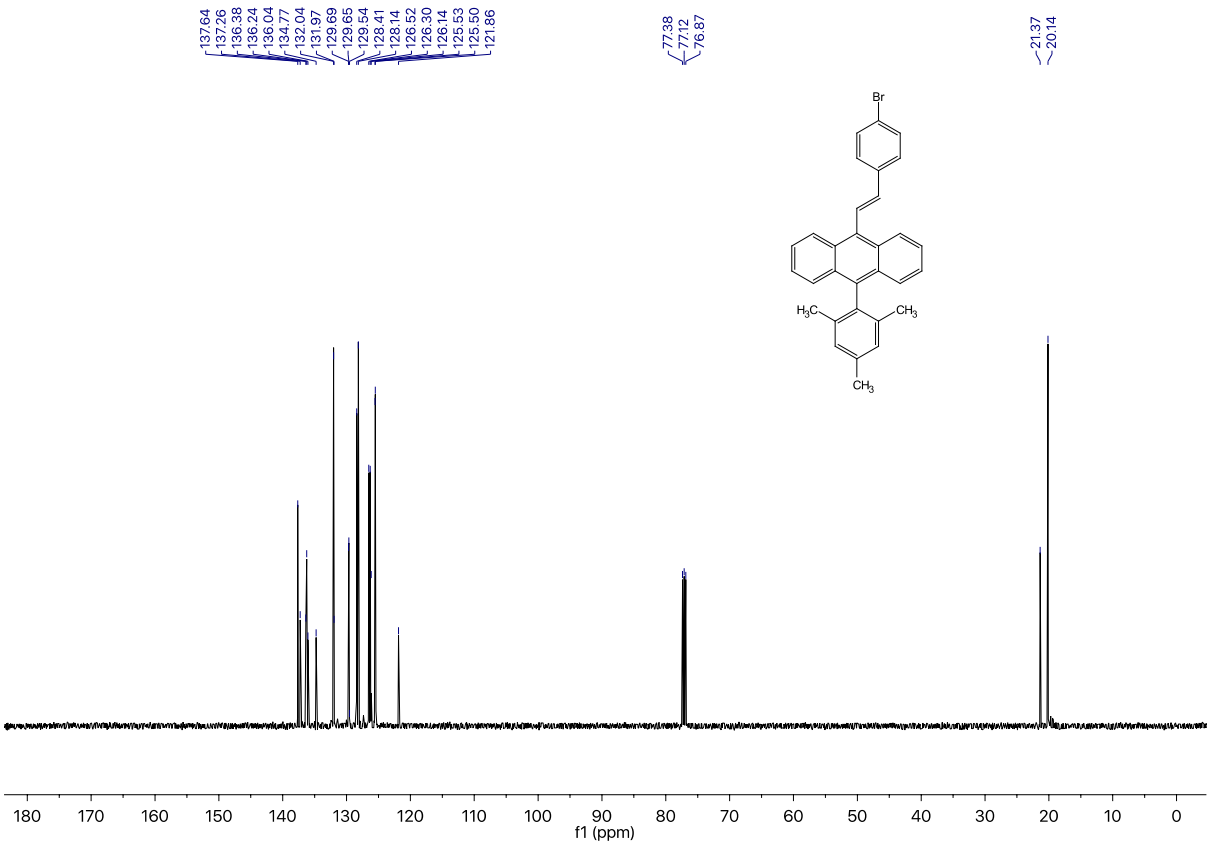

Fig S42 ^{13}C-NMR of compound **3a**

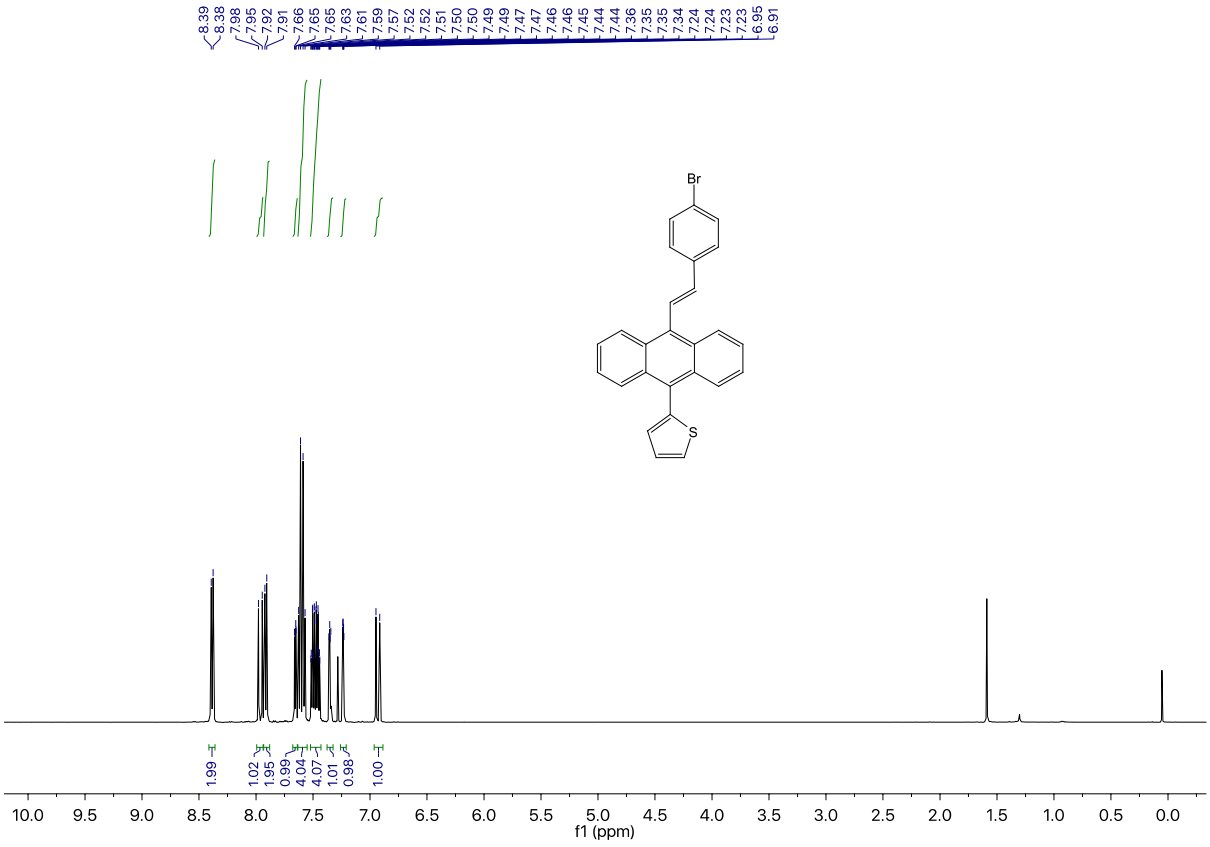

Fig S43 ^{1}H-NMR of compound **4a**

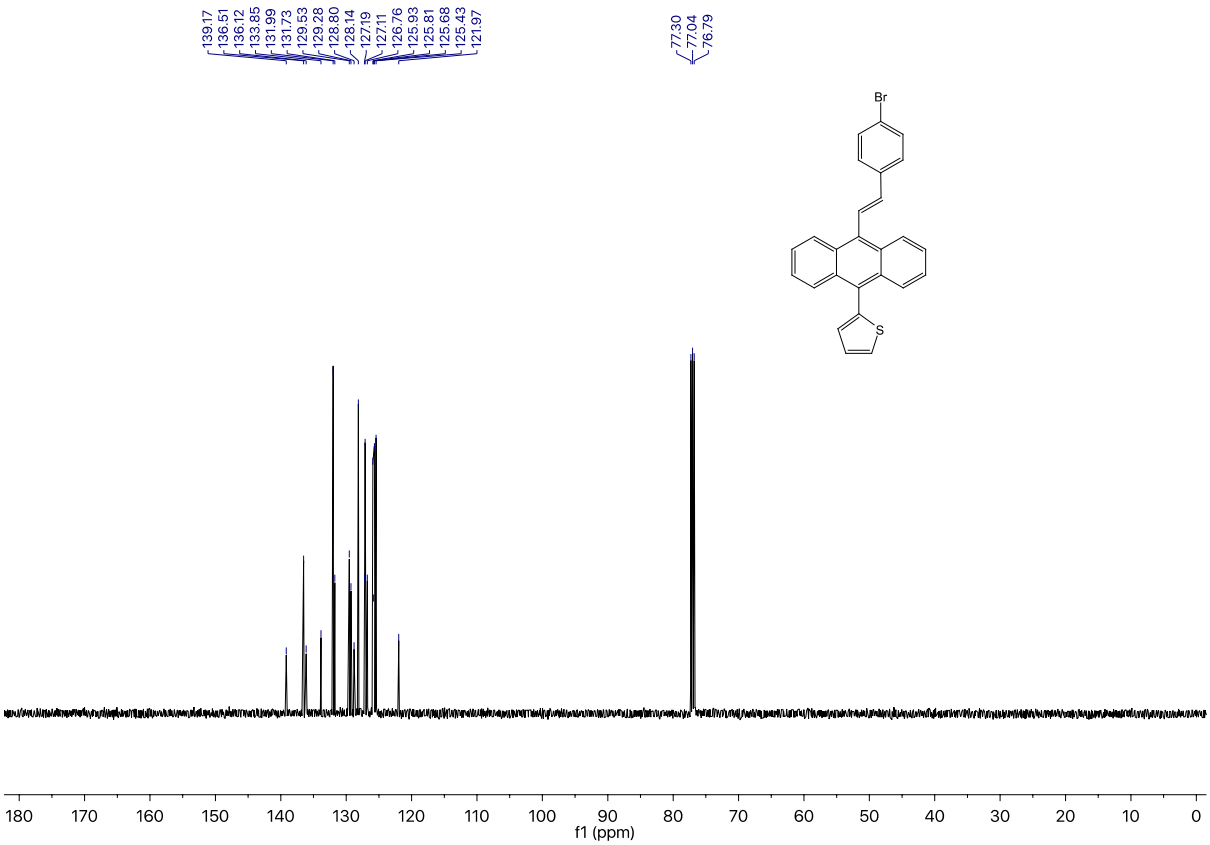

Fig S44 ^{13}C-NMR of compound **4a**

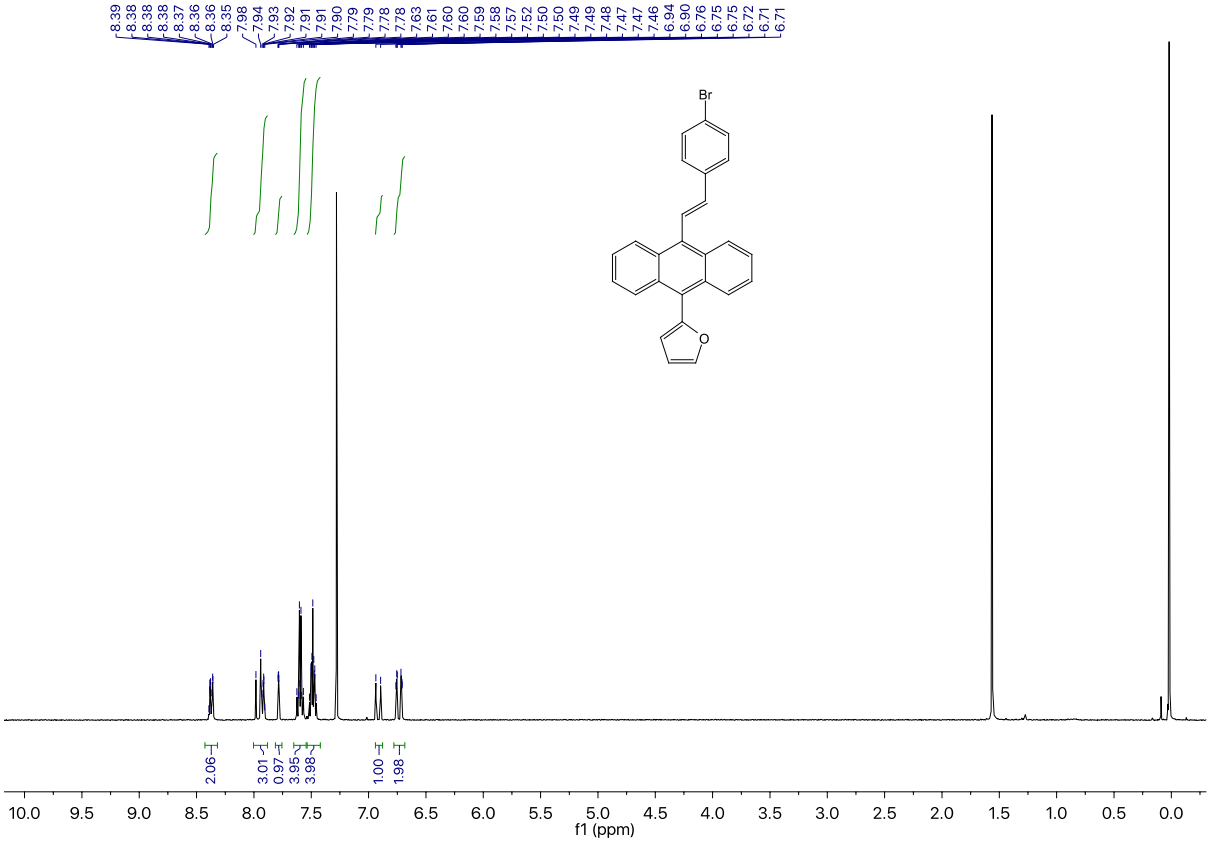

Fig S45 ^{1}H-NMR of compound **4b**

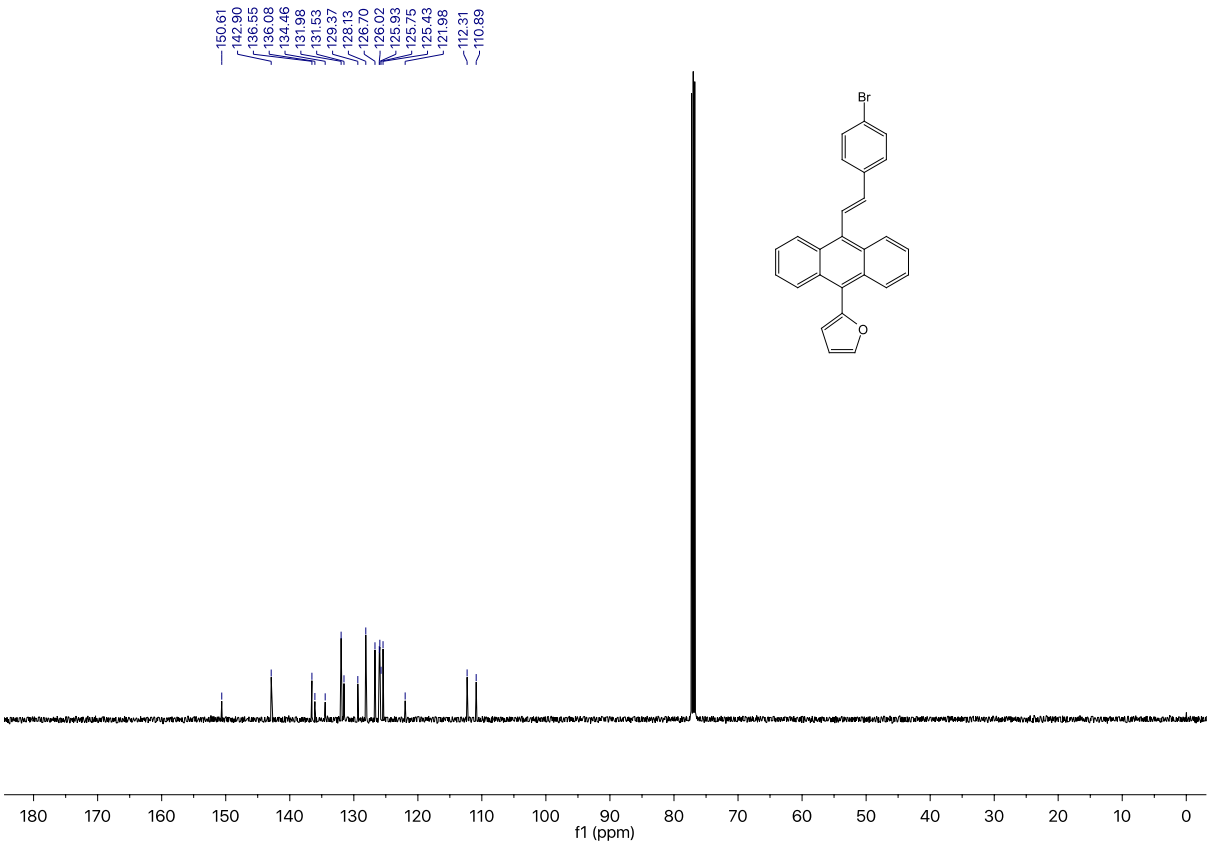

Fig S46 ^{13}C-NMR of compound **4b**

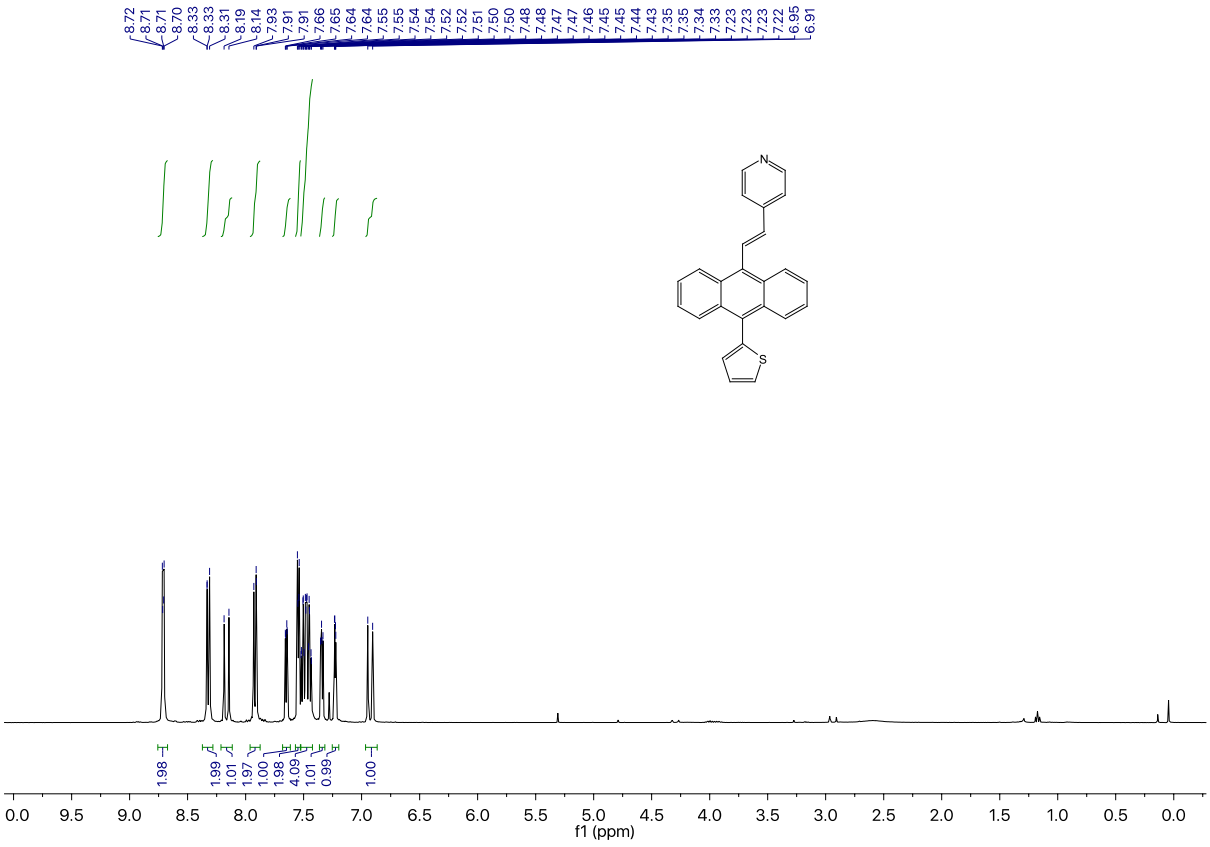

Fig S47 ^{1}H-NMR of compound **4c**

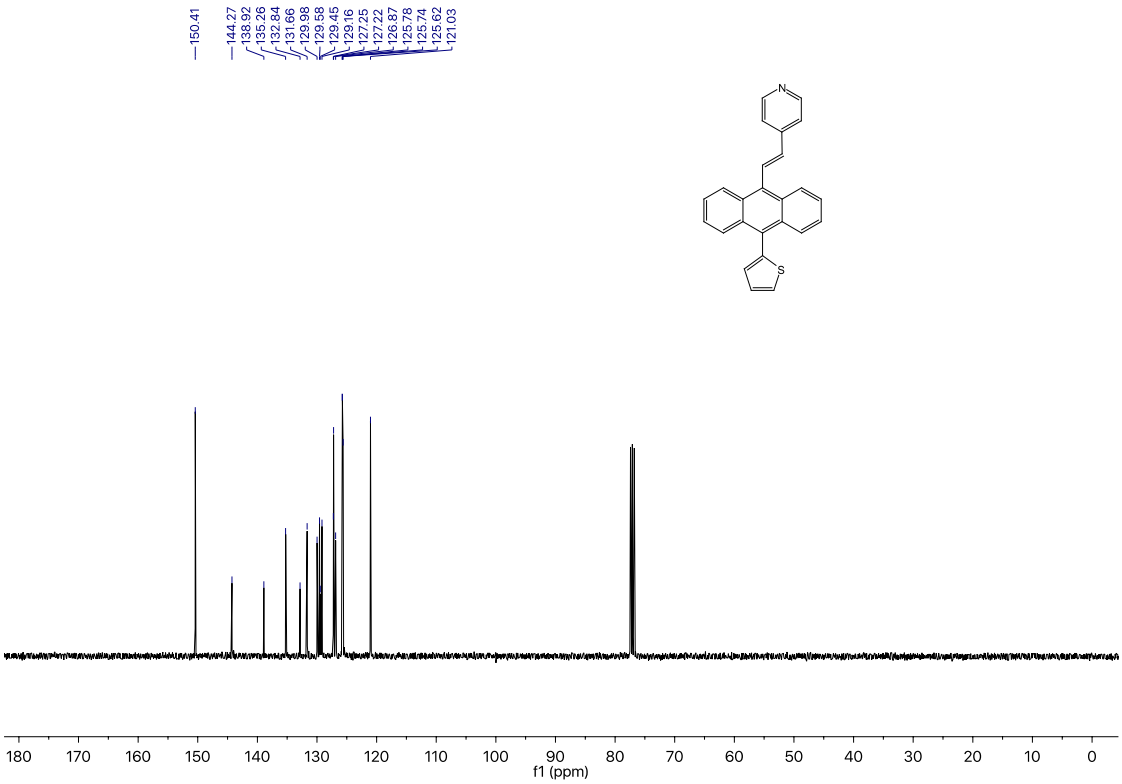

Fig S48 ^{13}C-NMR of compound **4c**

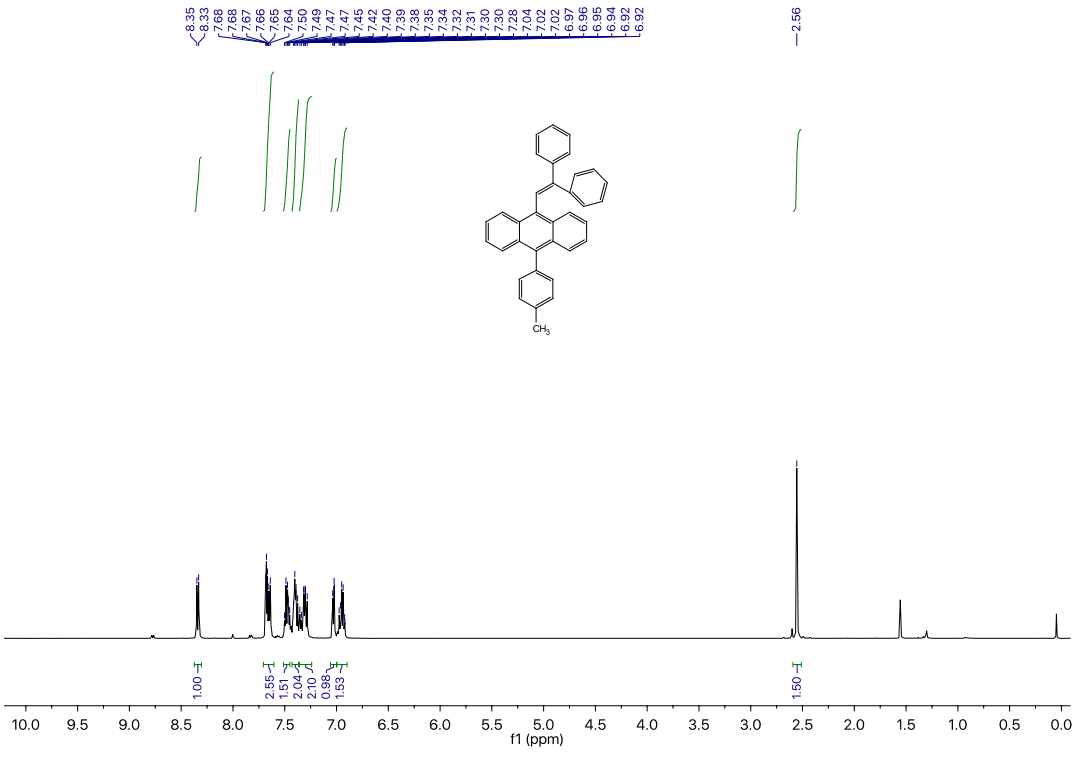

Fig S49 ^{1}H-NMR of compound **5**

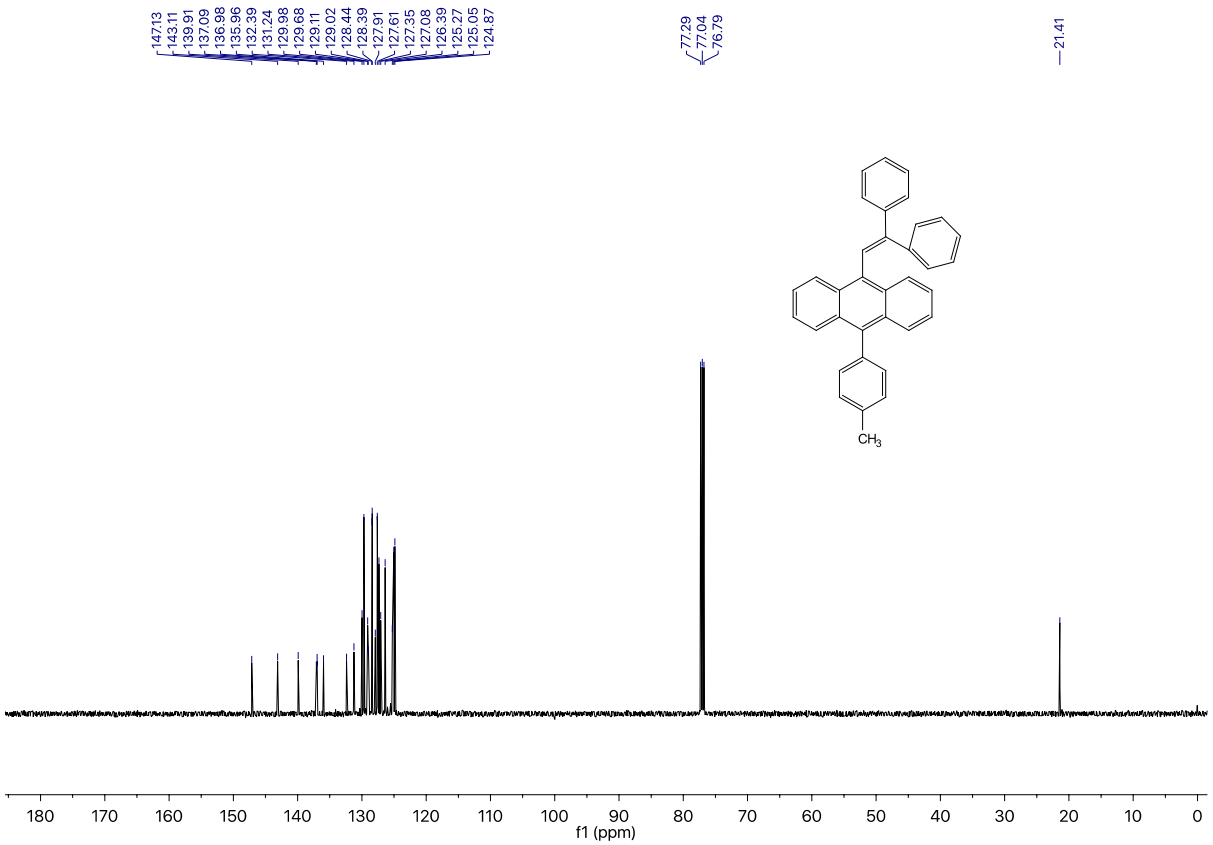

Fig S50 ^{13}C-NMR of compound **5**

_____End_____